

The Mechanistic Significance of the Si-O-Pd Bond in the Palladium Catalyzed Cross-Coupling Reactions of Arylsilanolates

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SUPPORTING INFORMATION: X-RAY DATA

Table of Contents	Page
X-Ray Crystal Structure and Analysis of 7e	S2
X-Ray Crystal Structure and Analysis of 7p	S17
X-Ray Crystal Structure and Analysis of 7z	S36
X-Ray Crystal Structure and Analysis of 7t	S52
X-Ray Crystal Structure and Analysis of 10	S70
X-Ray Crystal Structure and Analysis of 18	S86

X-Ray Crystal Structure of 7e (ga96pas)**Crystal Data and Structure Refinement for ga96pas:**

Identification code	ga96pas	
Empirical formula	C42 H44 O2 P2 Pd Si	
Formula weight	777.20	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 38.9379(14) Å b = 10.9293(5) Å c = 18.3057(8) Å	α= 90°. β= 99.210(3)°. γ = 90°.
Volume	7689.8(6) Å ³	
Z	8	
Density (calculated)	1.343 Mg/m ³	
Absorption coefficient	0.631 mm ⁻¹	
F(000)	3216	
Crystal size	0.50 x 0.12 x 0.08 mm ³	
Theta range for data collection	1.94 to 30.05°.	
Index ranges	-54<=h<=54, -14<=k<=15, -25<=l<=25	
Reflections collected	46758	
Independent reflections	11081 [R(int) = 0.0446]	
Completeness to theta = 30.05°	98.3 %	
Absorption correction	Integration	
Max. and min. transmission	0.9668 and 0.7818	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11081 / 0 / 437	
Goodness-of-fit on F ²	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0746	
R indices (all data)	R1 = 0.0713, wR2 = 0.0868	
Largest diff. peak and hole	0.598 and -0.385 e.Å ⁻³	

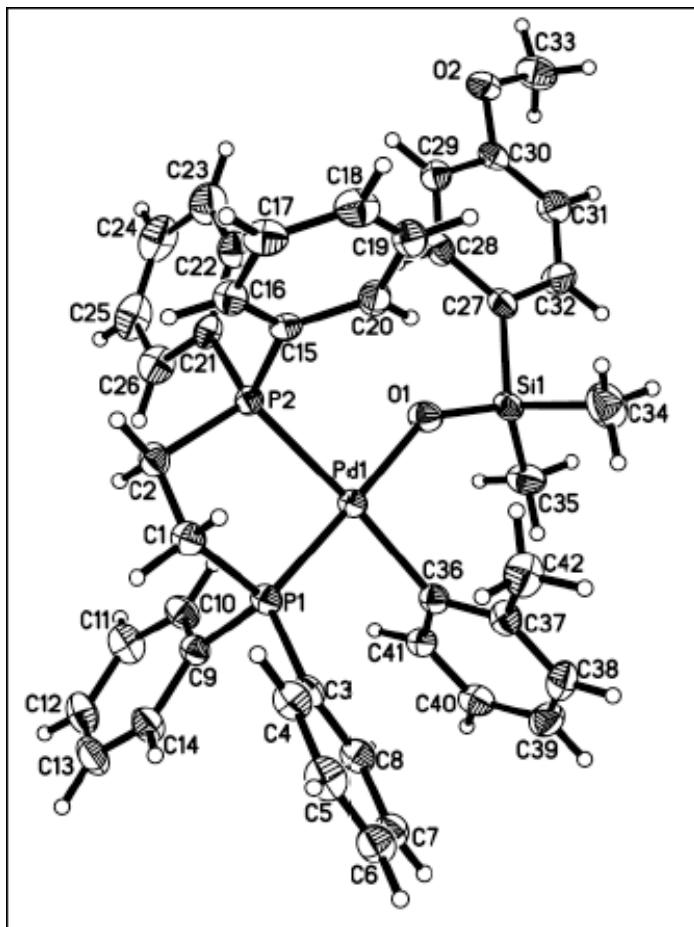


Figure 1. X-ray crystal structure of complex **7e**

The crystals were obtained directly from recrystallization as yellow needles $0.50 \times 0.12 \times 0.08$ mm in size and mounted using oil (Paratone-N, Exxon) to a 0.3 mm cryo-loop (Hampton Research) with the (9 1 3) scattering planes roughly normal to the spindle axis. Systematic absences for **7e** were consistent with the space group $C\bar{2}/c$. Unit cell dimensions were $a = 38.9379(14)$ Å, $b = 10.9293(5)$ Å, $c = 18.3057(8)$ Å, $\alpha = 90^\circ$, $\beta = 99.210^\circ$, $\gamma = 90^\circ$. Integration absorption correction was applied and maximum and minimum transmission factors were 0.9668 and 0.7818. The 11081 data points were used in the full-matrix least-squares refinement. The structure was solved using direct methods by using SHELXTL software package. Hydrogen

atoms were placed in “idealized” positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga96pas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	1376(1)	3431(2)	892(1)	38(1)
C(2)	1560(1)	3092(2)	1671(1)	39(1)
C(3)	803(1)	4775(2)	37(1)	32(1)
C(4)	971(1)	4542(2)	-565(1)	41(1)
C(5)	811(1)	4835(3)	-1272(2)	48(1)
C(6)	489(1)	5370(2)	-1387(2)	45(1)
C(7)	319(1)	5616(2)	-796(1)	39(1)
C(8)	475(1)	5317(2)	-87(1)	36(1)
C(9)	693(1)	3243(2)	1248(1)	32(1)
C(10)	667(1)	3097(2)	1986(1)	41(1)
C(11)	464(1)	2180(3)	2217(2)	52(1)
C(12)	283(1)	1403(3)	1709(2)	55(1)
C(13)	299(1)	1553(3)	969(2)	54(1)
C(14)	504(1)	2455(2)	737(2)	44(1)
C(15)	2035(1)	5147(2)	1950(1)	30(1)
C(16)	2279(1)	4461(2)	1649(1)	38(1)
C(17)	2571(1)	5026(3)	1453(2)	46(1)
C(18)	2623(1)	6261(3)	1563(2)	50(1)
C(19)	2385(1)	6941(3)	1872(2)	49(1)
C(20)	2090(1)	6401(2)	2055(1)	39(1)
C(21)	1758(1)	4038(2)	3175(1)	35(1)
C(22)	2033(1)	4572(2)	3637(2)	45(1)
C(23)	2104(1)	4283(3)	4386(2)	59(1)
C(24)	1898(1)	3458(3)	4675(2)	64(1)
C(25)	1624(1)	2924(3)	4228(2)	62(1)
C(26)	1550(1)	3212(3)	3481(2)	49(1)

C(27)	1517(1)	8467(2)	3909(1)	37(1)
C(28)	1776(1)	7627(2)	4161(1)	38(1)
C(29)	1993(1)	7752(2)	4832(1)	40(1)
C(30)	1954(1)	8738(2)	5282(1)	39(1)
C(31)	1702(1)	9586(3)	5056(2)	55(1)
C(32)	1488(1)	9444(3)	4377(2)	57(1)
C(33)	2106(1)	9713(3)	6447(2)	61(1)
C(34)	1315(1)	9625(3)	2417(2)	74(1)
C(35)	769(1)	8503(3)	3171(2)	53(1)
C(36)	720(1)	6743(2)	1464(1)	33(1)
C(37)	730(1)	7678(2)	959(1)	40(1)
C(38)	430(1)	8385(3)	742(2)	49(1)
C(39)	131(1)	8170(3)	1021(2)	50(1)
C(40)	118(1)	7227(3)	1516(2)	43(1)
C(41)	408(1)	6521(2)	1733(1)	35(1)
C(42)	1049(1)	7931(3)	623(2)	55(1)
O(1)	1315(1)	7002(2)	2664(1)	43(1)
O(2)	2174(1)	8775(2)	5954(1)	46(1)
P(1)	992(1)	4369(1)	977(1)	31(1)
P(2)	1641(1)	4504(1)	2211(1)	31(1)
Pd(1)	1156(1)	5758(1)	1845(1)	28(1)
Si(1)	1224(1)	8284(1)	2987(1)	36(1)

Table 2. Bond lengths [\AA] and angles [$^\circ$] for ga96pas.

C(1)-C(2)	1.534(3)
C(1)-P(1)	1.839(2)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-P(2)	1.832(2)
C(2)-H(2A)	0.9900
C(2)-H(30i)	0.9900
C(3)-C(4)	1.392(3)
C(3)-C(8)	1.392(3)
C(3)-P(1)	1.817(2)
C(4)-C(5)	1.380(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.371(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.382(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.383(3)
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(9)-C(10)	1.382(3)
C(9)-C(14)	1.393(3)
C(9)-P(1)	1.817(2)
C(10)-C(11)	1.383(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.368(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.376(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.376(4)
C(13)-H(13)	0.9500
C(14)-H(14)	0.9500
C(15)-C(16)	1.393(3)
C(15)-C(20)	1.395(3)
C(15)-P(2)	1.819(2)

C(16)-C(17)	1.389(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.374(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.379(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.379(3)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.383(4)
C(21)-C(26)	1.389(3)
C(21)-P(2)	1.823(3)
C(22)-C(23)	1.391(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.368(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.368(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.388(4)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(32)	1.385(3)
C(27)-C(28)	1.386(3)
C(27)-Si(1)	1.891(3)
C(28)-C(29)	1.383(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.379(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.365(4)
C(30)-O(2)	1.384(3)
C(31)-C(32)	1.390(4)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-O(2)	1.418(3)
C(33)-H(33A)	0.9800
C(33)-H(331i)	0.9800

C(33)-H(33C)	0.9800
C(34)-Si(1)	1.867(3)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-Si(1)	1.870(3)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.383(3)
C(36)-C(41)	1.405(3)
C(36)-Pd(1)	2.035(2)
C(37)-C(38)	1.403(3)
C(37)-C(42)	1.495(3)
C(38)-C(39)	1.366(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.378(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.374(3)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-H(42A)	0.9800
C(42)-H(430i)	0.9800
C(42)-H(42C)	0.9800
O(1)-Si(1)	1.5844(17)
O(1)-Pd(1)	2.0441(16)
P(1)-Pd(1)	2.2159(6)
P(2)-Pd(1)	2.3431(6)
C(2)-C(1)-P(1)	108.76(15)
C(2)-C(1)-H(1A)	109.9
P(1)-C(1)-H(1A)	109.9
C(2)-C(1)-H(1B)	109.9
P(1)-C(1)-H(1B)	109.9
H(1A)-C(1)-H(1B)	108.3
C(1)-C(2)-P(2)	108.18(16)

C(1)-C(2)-H(2A)	110.1
P(2)-C(2)-H(2A)	110.1
C(1)-C(2)-H(30i)	110.1
P(2)-C(2)-H(30i)	110.1
H(2A)-C(2)-H(30i)	108.4
C(4)-C(3)-C(8)	119.0(2)
C(4)-C(3)-P(1)	122.30(19)
C(8)-C(3)-P(1)	118.73(17)
C(5)-C(4)-C(3)	120.1(2)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	120.5(2)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	120.3(3)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	119.6(2)
C(6)-C(7)-H(7)	120.2
C(8)-C(7)-H(7)	120.2
C(7)-C(8)-C(3)	120.5(2)
C(7)-C(8)-H(8)	119.7
C(3)-C(8)-H(8)	119.7
C(10)-C(9)-C(14)	118.1(2)
C(10)-C(9)-P(1)	119.74(18)
C(14)-C(9)-P(1)	122.03(19)
C(9)-C(10)-C(11)	121.2(2)
C(9)-C(10)-H(10)	119.4
C(11)-C(10)-H(10)	119.4
C(12)-C(11)-C(10)	119.9(3)
C(12)-C(11)-H(11)	120.0
C(10)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	120.5(3)

C(12)-C(13)-H(13)	119.7
C(14)-C(13)-H(13)	119.7
C(13)-C(14)-C(9)	120.5(3)
C(13)-C(14)-H(14)	119.8
C(9)-C(14)-H(14)	119.8
C(16)-C(15)-C(20)	118.9(2)
C(16)-C(15)-P(2)	123.67(18)
C(20)-C(15)-P(2)	117.38(18)
C(17)-C(16)-C(15)	120.1(2)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(18)-C(17)-C(16)	120.3(2)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	119.8(2)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(20)	120.6(3)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(15)	120.1(2)
C(19)-C(20)-H(20)	119.9
C(15)-C(20)-H(20)	119.9
C(22)-C(21)-C(26)	118.1(2)
C(22)-C(21)-P(2)	121.62(19)
C(26)-C(21)-P(2)	120.0(2)
C(21)-C(22)-C(23)	121.3(3)
C(21)-C(22)-H(22)	119.3
C(23)-C(22)-H(22)	119.3
C(24)-C(23)-C(22)	119.6(3)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2
C(25)-C(24)-C(23)	120.0(3)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.7(3)

C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(25)-C(26)-C(21)	120.2(3)
C(25)-C(26)-H(26)	119.9
C(21)-C(26)-H(26)	119.9
C(32)-C(27)-C(28)	115.7(2)
C(32)-C(27)-Si(1)	122.3(2)
C(28)-C(27)-Si(1)	122.02(18)
C(29)-C(28)-C(27)	122.6(2)
C(29)-C(28)-H(28)	118.7
C(27)-C(28)-H(28)	118.7
C(30)-C(29)-C(28)	119.8(2)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	119.5(2)
C(31)-C(30)-O(2)	124.3(2)
C(29)-C(30)-O(2)	116.2(2)
C(30)-C(31)-C(32)	119.7(2)
C(30)-C(31)-H(31)	120.2
C(32)-C(31)-H(31)	120.2
C(27)-C(32)-C(31)	122.8(3)
C(27)-C(32)-H(32)	118.6
C(31)-C(32)-H(32)	118.6
O(2)-C(33)-H(33A)	109.5
O(2)-C(33)-H(331i)	109.5
H(33A)-C(33)-H(331i)	109.5
O(2)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(331i)-C(33)-H(33C)	109.5
Si(1)-C(34)-H(34A)	109.5
Si(1)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(1)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Si(1)-C(35)-H(35A)	109.5

Si(1)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
Si(1)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(37)-C(36)-C(41)	118.7(2)
C(37)-C(36)-Pd(1)	120.67(17)
C(41)-C(36)-Pd(1)	120.59(18)
C(36)-C(37)-C(38)	119.0(2)
C(36)-C(37)-C(42)	121.6(2)
C(38)-C(37)-C(42)	119.3(2)
C(39)-C(38)-C(37)	121.4(3)
C(39)-C(38)-H(38)	119.3
C(37)-C(38)-H(38)	119.3
C(38)-C(39)-C(40)	119.8(2)
C(38)-C(39)-H(39)	120.1
C(40)-C(39)-H(39)	120.1
C(41)-C(40)-C(39)	119.7(2)
C(41)-C(40)-H(40)	120.1
C(39)-C(40)-H(40)	120.1
C(40)-C(41)-C(36)	121.3(2)
C(40)-C(41)-H(41)	119.3
C(36)-C(41)-H(41)	119.3
C(37)-C(42)-H(42A)	109.5
C(37)-C(42)-H(430i)	109.5
H(42A)-C(42)-H(430i)	109.5
C(37)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(430i)-C(42)-H(42C)	109.5
Si(1)-O(1)-Pd(1)	143.39(10)
C(30)-O(2)-C(33)	115.7(2)
C(9)-P(1)-C(3)	104.05(11)
C(9)-P(1)-C(1)	102.18(11)
C(3)-P(1)-C(1)	105.57(11)
C(9)-P(1)-Pd(1)	113.05(8)
C(3)-P(1)-Pd(1)	122.59(8)

C(1)-P(1)-Pd(1)	107.37(8)
C(15)-P(2)-C(21)	105.70(11)
C(15)-P(2)-C(2)	105.20(11)
C(21)-P(2)-C(2)	106.39(11)
C(15)-P(2)-Pd(1)	111.99(8)
C(21)-P(2)-Pd(1)	120.34(7)
C(2)-P(2)-Pd(1)	106.14(8)
C(36)-Pd(1)-O(1)	92.17(8)
C(36)-Pd(1)-P(1)	89.35(7)
O(1)-Pd(1)-P(1)	178.36(5)
C(36)-Pd(1)-P(2)	175.32(7)
O(1)-Pd(1)-P(2)	92.51(5)
P(1)-Pd(1)-P(2)	85.97(2)
O(1)-Si(1)-C(34)	114.26(14)
O(1)-Si(1)-C(35)	117.13(11)
C(34)-Si(1)-C(35)	105.72(16)
O(1)-Si(1)-C(27)	106.71(10)
C(34)-Si(1)-C(27)	105.88(14)
C(35)-Si(1)-C(27)	106.35(12)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga96pas. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	33(1)	40(1)	42(2)	-13(1)	11(1)	4(1)
C(2)	32(1)	32(1)	54(2)	-7(1)	12(1)	3(1)
C(3)	37(1)	31(1)	30(1)	-8(1)	8(1)	-5(1)
C(4)	45(1)	45(2)	36(2)	-7(1)	17(1)	-2(1)
C(5)	61(2)	52(2)	35(2)	-5(1)	23(1)	-5(1)
C(6)	57(2)	45(2)	33(2)	-1(1)	9(1)	-7(1)
C(7)	43(1)	38(1)	37(1)	-2(1)	6(1)	-2(1)
C(8)	38(1)	39(1)	33(1)	-8(1)	11(1)	-2(1)
C(9)	32(1)	32(1)	33(1)	-6(1)	8(1)	1(1)
C(10)	41(1)	43(2)	41(2)	-11(1)	12(1)	-6(1)

C(11)	65(2)	53(2)	43(2)	-3(1)	22(1)	-9(2)
C(12)	64(2)	39(2)	67(2)	-2(1)	22(2)	-12(1)
C(13)	68(2)	37(2)	56(2)	-9(1)	4(2)	-13(1)
C(14)	55(2)	37(1)	40(2)	-5(1)	7(1)	-7(1)
C(15)	28(1)	36(1)	26(1)	1(1)	2(1)	1(1)
C(16)	35(1)	41(2)	37(1)	-5(1)	9(1)	1(1)
C(17)	35(1)	62(2)	42(2)	-5(1)	14(1)	0(1)
C(18)	40(1)	65(2)	47(2)	12(1)	12(1)	-10(1)
C(19)	48(2)	40(2)	58(2)	10(1)	5(1)	-5(1)
C(20)	39(1)	35(1)	44(2)	2(1)	7(1)	2(1)
C(21)	37(1)	33(1)	38(1)	4(1)	12(1)	9(1)
C(22)	54(2)	41(2)	39(2)	2(1)	10(1)	1(1)
C(23)	79(2)	56(2)	40(2)	3(1)	3(2)	5(2)
C(24)	94(3)	68(2)	35(2)	11(2)	20(2)	22(2)
C(25)	70(2)	61(2)	63(2)	21(2)	38(2)	9(2)
C(26)	44(2)	54(2)	54(2)	8(1)	20(1)	2(1)
C(27)	33(1)	34(1)	44(2)	-10(1)	8(1)	-5(1)
C(28)	40(1)	33(1)	44(2)	-8(1)	16(1)	-2(1)
C(29)	36(1)	41(1)	45(2)	-1(1)	12(1)	2(1)
C(30)	34(1)	41(1)	41(2)	-2(1)	8(1)	-12(1)
C(31)	54(2)	48(2)	59(2)	-27(1)	-7(2)	9(1)
C(32)	53(2)	48(2)	62(2)	-25(1)	-11(2)	17(1)
C(33)	63(2)	72(2)	47(2)	-16(2)	-1(2)	-9(2)
C(34)	97(3)	63(2)	62(2)	7(2)	12(2)	-21(2)
C(35)	38(1)	60(2)	61(2)	-21(2)	5(1)	4(1)
C(36)	33(1)	34(1)	32(1)	-7(1)	6(1)	1(1)
C(37)	42(1)	38(1)	43(2)	-5(1)	13(1)	0(1)
C(38)	55(2)	40(2)	53(2)	4(1)	9(1)	11(1)
C(39)	46(2)	48(2)	53(2)	-2(1)	2(1)	13(1)
C(40)	33(1)	50(2)	48(2)	-12(1)	10(1)	0(1)
C(41)	33(1)	38(1)	34(1)	-4(1)	6(1)	1(1)
C(42)	55(2)	56(2)	58(2)	11(2)	25(1)	0(1)
O(1)	38(1)	46(1)	43(1)	-19(1)	1(1)	5(1)
O(2)	44(1)	53(1)	40(1)	-4(1)	1(1)	-9(1)
P(1)	28(1)	34(1)	32(1)	-8(1)	9(1)	1(1)
P(2)	28(1)	31(1)	34(1)	-1(1)	8(1)	2(1)

Pd(1)	25(1)	30(1)	29(1)	-6(1)	7(1)	1(1)
Si(1)	33(1)	35(1)	40(1)	-10(1)	7(1)	-3(1)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga96pas.

Atom	x	y	z	U(eq)
H(1A)	1304	2680	607	45
H(1B)	1537	3895	627	45
H(2A)	1783	2675	1640	46
H(30i)	1413	2532	1911	46
H(4)	1196	4180	-489	49
H(5)	926	4666	-1681	57
H(6)	382	5571	-1875	54
H(7)	95	5989	-877	47
H(8)	358	5484	320	43
H(10)	790	3637	2342	49
H(11)	451	2088	2728	62
H(12)	147	764	1866	66
H(13)	168	1030	615	65
H(14)	516	2540	225	53
H(16)	2247	3606	1577	45
H(17)	2736	4557	1242	55
H(18)	2822	6644	1426	60
H(19)	2424	7790	1960	59
H(20)	1924	6883	2253	47
H(22)	2177	5147	3439	53
H(23)	2295	4656	4695	71
H(24)	1945	3257	5186	77
H(25)	1482	2349	4431	75
H(26)	1357	2844	3178	59
H(28)	1805	6938	3861	45
H(29)	2169	7161	4984	48

H(31)	1673	10269	5361	66
H(32)	1314	10043	4227	68
H(33A)	2264	9626	6918	92
H(331i)	1865	9650	6534	92
H(33C)	2142	10513	6229	92
H(34A)	1147	9640	1956	111
H(34B)	1551	9558	2300	111
H(34C)	1295	10382	2694	111
H(35A)	609	8528	2700	80
H(35B)	754	9274	3437	80
H(35C)	706	7822	3471	80
H(38)	436	9026	394	59
H(39)	-68	8669	873	59
H(40)	-91	7066	1705	52
H(41)	397	5870	2073	42
H(42A)	1252	7966	1015	82
H(430i)	1022	8716	362	82
H(42C)	1080	7278	274	82

X-Ray crystal structure of 7p (g39jas).**Crystal data and structure refinement for g39jas.**

Identification code	g39jas		
Empirical formula	C52 H55 O2 P2 Pd Si		
Formula weight	908.39		
Temperature	193(2) K		
Wavelength	0.71073 Å		
Crystal system	Triclinic		
Space group	P -1		
Unit cell dimensions	$a = 10.3193(6)$ Å	$\alpha = 93.3770(10)^\circ$.	
	$b = 10.8718(6)$ Å	$\beta = 96.2100(10)^\circ$.	
	$c = 20.9256(11)$ Å	$\gamma = 95.5570(10)^\circ$.	
Volume	$2317.2(2)$ Å ³		
Z	2		
Density (calculated)	1.302 Mg/m ³		
Absorption coefficient	0.534 mm ⁻¹		
F(000)	946		
Crystal size	0.36 x 0.26 x 0.08 mm ³		
Theta range for data collection	2.00 to 25.39°.		
Index ranges	-12≤h≤12, -13≤k≤13, -25≤l≤25		
Reflections collected	24188		
Independent reflections	8499 [R(int) = 0.0368]		
Completeness to theta = 25.39°	99.7 %		
Absorption correction	Integration		
Max. and min. transmission	0.9565 and 0.8415		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	8499 / 228 / 573		
Goodness-of-fit on F ²	1.048		
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0731		
R indices (all data)	R1 = 0.0479, wR2 = 0.0777		
Largest diff. peak and hole	0.402 and -0.275 e.Å ⁻³		

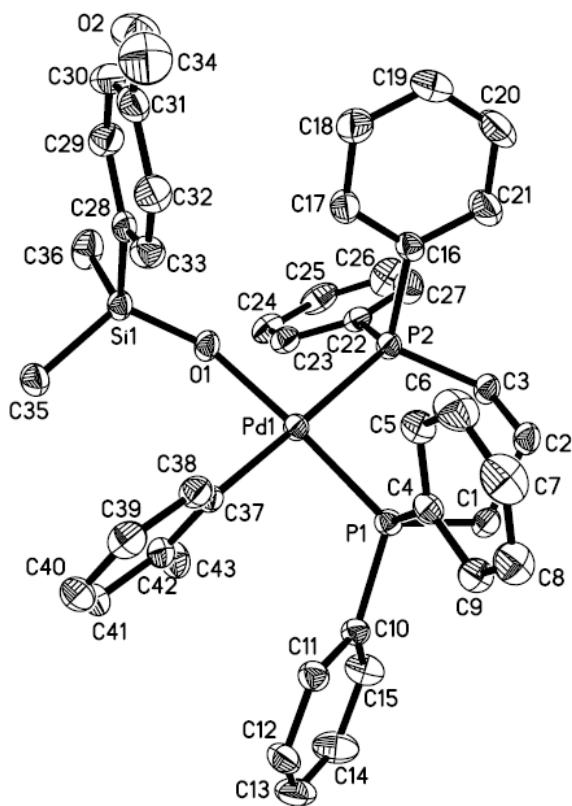


Figure 2. X-ray structure of complex **7p**.

The crystals were obtained directly from recrystallization as yellow needles 0.36 x 0.26 x 0.08 mm in size and mounted using oil (Parantone-N, Exxon) to a thin glass fiber with the (1 0 0) scattering planes roughly normal to the spindle axis. Systematic absences for **7p** were consistent with the space group P-1. Unit cell dimensions were $a = 10.3193(6)$ Å, $b = 10.8718(6)$ Å, $c = 20.9256(11)$ Å, $\alpha = 93.3770(10)^\circ$, $\beta = 96.2100(10)^\circ$, $\gamma = 95.5570(10)^\circ$. Integration absorption correction was applied (absorption coefficient $\mu = 0.534$ mm⁻¹), and maximum and minimum transmission factors were 0.9565 and 0.8415. The 8499 data points were used in the full-matrix least-squares refinement. The structure was solved using direct methods by using SHELXTL

software package. Hydrogen atoms were placed in “idealized” positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for g39jas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	5213(2)	3067(2)	2076(1)	35(1)
C(2)	5897(2)	3916(2)	2647(1)	37(1)
C(3)	5977(2)	5283(2)	2513(1)	35(1)
C(4)	3089(2)	2018(2)	2664(1)	32(1)
C(5)	2694(3)	2558(3)	3218(1)	42(1)
C(6)	2522(3)	1860(3)	3743(2)	60(1)
C(7)	2728(3)	631(3)	3709(2)	63(1)
C(8)	3118(3)	89(3)	3163(2)	53(1)
C(9)	3306(3)	776(2)	2646(1)	40(1)
C(10)	2959(2)	1961(2)	1259(1)	32(1)
C(11)	1864(3)	1093(2)	1195(1)	35(1)
C(12)	1491(3)	406(3)	611(1)	45(1)
C(13)	2180(3)	585(3)	96(1)	54(1)
C(14)	3258(3)	1443(3)	153(2)	60(1)
C(15)	3647(3)	2134(3)	730(1)	46(1)
C(16)	4336(2)	6461(2)	3366(1)	33(1)
C(17)	3139(3)	6755(3)	3532(1)	41(1)
C(18)	3008(3)	7185(3)	4153(1)	51(1)
C(19)	4056(3)	7304(3)	4620(2)	56(1)
C(20)	5244(3)	6980(4)	4465(2)	71(1)
C(21)	5382(3)	6564(3)	3842(2)	62(1)
C(22)	4831(2)	7421(2)	2145(1)	32(1)
C(23)	3983(3)	7783(2)	1646(1)	36(1)
C(24)	4346(3)	8805(2)	1313(1)	44(1)
C(25)	5551(3)	9465(3)	1474(2)	52(1)
C(26)	6391(3)	9140(3)	1975(2)	59(1)

C(27)	6036(3)	8121(3)	2312(2)	49(1)
C(28)	-342(2)	6713(2)	2975(1)	34(1)
C(29)	-534(3)	7724(3)	3388(1)	45(1)
C(30)	-920(3)	7583(3)	3994(1)	48(1)
C(31)	-1130(3)	6424(3)	4215(1)	43(1)
C(32)	-952(3)	5401(3)	3830(1)	46(1)
C(33)	-569(3)	5563(3)	3225(1)	42(1)
C(34)	-1957(4)	5208(3)	5028(2)	72(1)
C(35)	-1209(2)	6085(3)	1560(1)	41(1)
C(36)	338(3)	8514(3)	1973(2)	52(1)
C(37)	813(2)	3665(2)	1677(1)	29(1)
C(38)	9(2)	2999(2)	2060(1)	38(1)
C(39)	-1185(3)	2369(2)	1793(2)	48(1)
C(40)	-1570(3)	2391(3)	1146(2)	53(1)
C(41)	-788(3)	3023(3)	760(2)	47(1)
C(42)	415(2)	3676(2)	1019(1)	37(1)
C(43)	1241(3)	4381(3)	590(1)	49(1)
O(1)	1543(2)	6291(2)	2088(1)	34(1)
O(2)	-1514(2)	6388(2)	4827(1)	61(1)
P(1)	3417(1)	2968(1)	1998(1)	28(1)
P(2)	4428(1)	5973(1)	2520(1)	30(1)
Pd(1)	2508(1)	4728(1)	2058(1)	27(1)
Si(1)	178(1)	6837(1)	2139(1)	32(1)
C(44)	878(8)	8594(11)	5654(5)	67(2)
C(45)	1728(10)	9264(11)	5299(4)	60(2)
C(46)	2966(9)	9745(11)	5585(5)	62(2)
C(47)	3353(7)	9557(12)	6226(5)	70(2)
C(48)	2503(12)	8887(10)	6581(4)	81(3)
C(49)	1265(12)	8406(9)	6294(4)	78(2)
C(50)	5491(15)	5617(12)	572(8)	27(2)
C(51)	6244(15)	4691(13)	391(9)	33(2)
C(52)	5844(16)	3932(13)	-167(9)	35(2)
C(53)	4689(16)	4100(12)	-545(8)	34(2)
C(54)	3936(16)	5026(12)	-364(8)	31(2)
C(55)	4336(15)	5785(12)	194(8)	31(2)
C(56)	1175(5)	8312(6)	5738(3)	68(2)

C(57)	1540(6)	9203(7)	5324(3)	62(2)
C(58)	2713(6)	9959(6)	5471(3)	62(2)
C(59)	3520(4)	9825(5)	6033(3)	66(2)
C(60)	3155(8)	8935(5)	6448(3)	76(2)
C(61)	1983(9)	8178(5)	6301(3)	82(2)

Table 6. Bond lengths [\AA] and angles [$^\circ$] for g39jas.

C(1)-C(2)	1.529(3)
C(1)-P(1)	1.835(2)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.524(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-P(2)	1.832(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.388(4)
C(4)-C(9)	1.389(4)
C(4)-P(1)	1.823(3)
C(5)-C(6)	1.388(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.373(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.372(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(4)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(3)
C(10)-C(15)	1.391(4)
C(10)-P(1)	1.833(2)

C(11)-C(12)	1.392(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.366(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.371(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.382(4)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.378(4)
C(16)-C(17)	1.380(4)
C(16)-P(2)	1.834(3)
C(17)-C(18)	1.381(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.368(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.374(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.381(4)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.389(4)
C(22)-C(27)	1.392(3)
C(22)-P(2)	1.831(3)
C(23)-C(24)	1.389(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.372(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.372(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.389(4)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(33)	1.393(4)
C(28)-C(29)	1.401(4)
C(28)-Si(1)	1.893(3)

C(29)-C(30)	1.381(4)
C(29)-H(29)	0.9500
C(30)-C(31)	1.374(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.374(4)
C(31)-O(2)	1.382(3)
C(32)-C(33)	1.381(4)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-O(2)	1.423(4)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-Si(1)	1.862(3)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-Si(1)	1.871(3)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(42)	1.395(4)
C(37)-C(38)	1.397(3)
C(37)-Pd(1)	2.057(2)
C(38)-C(39)	1.393(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.372(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.370(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.406(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.497(4)
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800

O(1)-Si(1)	1.5918(17)
O(1)-Pd(1)	2.0522(16)
P(1)-Pd(1)	2.2143(7)
P(2)-Pd(1)	2.3671(6)
C(44)-C(45)	1.3900
C(44)-C(49)	1.3900
C(44)-H(44)	0.9500
C(45)-C(46)	1.3900
C(45)-H(45)	0.9500
C(46)-C(47)	1.3900
C(46)-H(46)	0.9500
C(47)-C(48)	1.3900
C(47)-H(47)	0.9500
C(48)-C(49)	1.3900
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(51)	1.3900
C(50)-C(55)	1.3900
C(50)-H(50)	0.9500
C(51)-C(52)	1.3900
C(51)-H(51)	0.9500
C(52)-C(53)	1.3900
C(52)-H(52)	0.9500
C(53)-C(54)	1.3900
C(53)-H(53)	0.9500
C(54)-C(55)	1.3900
C(54)-H(54)	0.9500
C(55)-H(55)	0.9500
C(56)-C(57)	1.3900
C(56)-C(61)	1.3900
C(56)-H(56)	0.9500
C(57)-C(58)	1.3900
C(57)-H(57)	0.9500
C(58)-C(59)	1.3900
C(58)-H(58)	0.9500
C(59)-C(60)	1.3900

C(59)-H(59)	0.9500
C(60)-C(61)	1.3900
C(60)-H(60)	0.9500
C(61)-H(61)	0.9500
C(2)-C(1)-P(1)	114.48(18)
C(2)-C(1)-H(1A)	108.6
P(1)-C(1)-H(1A)	108.6
C(2)-C(1)-H(1B)	108.6
P(1)-C(1)-H(1B)	108.6
H(1A)-C(1)-H(1B)	107.6
C(3)-C(2)-C(1)	112.9(2)
C(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2A)	109.0
C(3)-C(2)-H(2B)	109.0
C(1)-C(2)-H(2B)	109.0
H(2A)-C(2)-H(2B)	107.8
C(2)-C(3)-P(2)	114.69(17)
C(2)-C(3)-H(3A)	108.6
P(2)-C(3)-H(3A)	108.6
C(2)-C(3)-H(3B)	108.6
P(2)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(5)-C(4)-C(9)	118.8(2)
C(5)-C(4)-P(1)	119.7(2)
C(9)-C(4)-P(1)	121.3(2)
C(4)-C(5)-C(6)	120.2(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(7)-C(6)-C(5)	119.8(3)
C(7)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(8)-C(7)-C(6)	120.5(3)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	120.0(3)
C(9)-C(8)-H(8)	120.0

C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(4)	120.7(3)
C(8)-C(9)-H(9)	119.6
C(4)-C(9)-H(9)	119.6
C(11)-C(10)-C(15)	118.8(2)
C(11)-C(10)-P(1)	121.2(2)
C(15)-C(10)-P(1)	119.72(19)
C(10)-C(11)-C(12)	119.7(3)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	120.7(3)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(12)-C(13)-C(14)	120.1(3)
C(12)-C(13)-H(13)	120.0
C(14)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.1(3)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-C(10)	120.6(3)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7
C(21)-C(16)-C(17)	118.4(3)
C(21)-C(16)-P(2)	124.3(2)
C(17)-C(16)-P(2)	117.32(19)
C(16)-C(17)-C(18)	120.6(3)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	120.7(3)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	119.1(3)
C(18)-C(19)-H(19)	120.4
C(20)-C(19)-H(19)	120.4
C(19)-C(20)-C(21)	120.4(3)
C(19)-C(20)-H(20)	119.8

C(21)-C(20)-H(20)	119.8
C(16)-C(21)-C(20)	120.8(3)
C(16)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(23)-C(22)-C(27)	118.5(2)
C(23)-C(22)-P(2)	120.20(19)
C(27)-C(22)-P(2)	121.0(2)
C(24)-C(23)-C(22)	120.5(3)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(25)-C(24)-C(23)	120.1(3)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(24)-C(25)-C(26)	120.3(3)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	120.0(3)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(26)-C(27)-C(22)	120.6(3)
C(26)-C(27)-H(27)	119.7
C(22)-C(27)-H(27)	119.7
C(33)-C(28)-C(29)	114.6(3)
C(33)-C(28)-Si(1)	120.8(2)
C(29)-C(28)-Si(1)	124.6(2)
C(30)-C(29)-C(28)	122.4(3)
C(30)-C(29)-H(29)	118.8
C(28)-C(29)-H(29)	118.8
C(31)-C(30)-C(29)	120.5(3)
C(31)-C(30)-H(30)	119.8
C(29)-C(30)-H(30)	119.8
C(32)-C(31)-C(30)	119.5(3)
C(32)-C(31)-O(2)	124.7(3)
C(30)-C(31)-O(2)	115.8(3)
C(31)-C(32)-C(33)	119.1(3)
C(31)-C(32)-H(32)	120.5

C(33)-C(32)-H(32)	120.5
C(32)-C(33)-C(28)	124.0(3)
C(32)-C(33)-H(33)	118.0
C(28)-C(33)-H(33)	118.0
O(2)-C(34)-H(34A)	109.5
O(2)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
O(2)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Si(1)-C(35)-H(35A)	109.5
Si(1)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
Si(1)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
Si(1)-C(36)-H(36A)	109.5
Si(1)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
Si(1)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(42)-C(37)-C(38)	119.1(2)
C(42)-C(37)-Pd(1)	118.50(18)
C(38)-C(37)-Pd(1)	122.27(19)
C(39)-C(38)-C(37)	120.7(3)
C(39)-C(38)-H(38)	119.7
C(37)-C(38)-H(38)	119.7
C(40)-C(39)-C(38)	119.7(3)
C(40)-C(39)-H(39)	120.1
C(38)-C(39)-H(39)	120.1
C(41)-C(40)-C(39)	120.5(3)
C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7
C(40)-C(41)-C(42)	120.8(3)
C(40)-C(41)-H(41)	119.6

C(42)-C(41)-H(41)	119.6
C(37)-C(42)-C(41)	119.1(3)
C(37)-C(42)-C(43)	121.0(2)
C(41)-C(42)-C(43)	119.9(3)
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
Si(1)-O(1)-Pd(1)	146.22(10)
C(31)-O(2)-C(34)	117.3(2)
C(4)-P(1)-C(10)	106.28(11)
C(4)-P(1)-C(1)	100.26(12)
C(10)-P(1)-C(1)	102.14(12)
C(4)-P(1)-Pd(1)	112.11(9)
C(10)-P(1)-Pd(1)	116.73(8)
C(1)-P(1)-Pd(1)	117.43(8)
C(22)-P(2)-C(3)	100.59(12)
C(22)-P(2)-C(16)	104.25(11)
C(3)-P(2)-C(16)	105.40(12)
C(22)-P(2)-Pd(1)	116.55(9)
C(3)-P(2)-Pd(1)	116.73(8)
C(16)-P(2)-Pd(1)	111.81(8)
O(1)-Pd(1)-C(37)	91.17(8)
O(1)-Pd(1)-P(1)	175.99(5)
C(37)-Pd(1)-P(1)	84.82(7)
O(1)-Pd(1)-P(2)	87.85(5)
C(37)-Pd(1)-P(2)	178.39(7)
P(1)-Pd(1)-P(2)	96.15(2)
O(1)-Si(1)-C(35)	115.02(11)
O(1)-Si(1)-C(36)	109.59(12)
C(35)-Si(1)-C(36)	106.00(13)
O(1)-Si(1)-C(28)	111.12(10)
C(35)-Si(1)-C(28)	106.91(12)
C(36)-Si(1)-C(28)	107.86(13)

C(45)-C(44)-C(49)	120.0
C(45)-C(44)-H(44)	120.0
C(49)-C(44)-H(44)	120.0
C(46)-C(45)-C(44)	120.0
C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0
C(45)-C(46)-C(47)	120.0
C(45)-C(46)-H(46)	120.0
C(47)-C(46)-H(46)	120.0
C(48)-C(47)-C(46)	120.0
C(48)-C(47)-H(47)	120.0
C(46)-C(47)-H(47)	120.0
C(47)-C(48)-C(49)	120.0
C(47)-C(48)-H(48)	120.0
C(49)-C(48)-H(48)	120.0
C(48)-C(49)-C(44)	120.0
C(48)-C(49)-H(49)	120.0
C(44)-C(49)-H(49)	120.0
C(51)-C(50)-C(55)	120.0
C(51)-C(50)-H(50)	120.0
C(55)-C(50)-H(50)	120.0
C(52)-C(51)-C(50)	120.0
C(52)-C(51)-H(51)	120.0
C(50)-C(51)-H(51)	120.0
C(53)-C(52)-C(51)	120.0
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0
C(52)-C(53)-C(54)	120.0
C(52)-C(53)-H(53)	120.0
C(54)-C(53)-H(53)	120.0
C(53)-C(54)-C(55)	120.0
C(53)-C(54)-H(54)	120.0
C(55)-C(54)-H(54)	120.0
C(54)-C(55)-C(50)	120.0
C(54)-C(55)-H(55)	120.0
C(50)-C(55)-H(55)	120.0

C(57)-C(56)-C(61)	120.0
C(57)-C(56)-H(56)	120.0
C(61)-C(56)-H(56)	120.0
C(56)-C(57)-C(58)	120.0
C(56)-C(57)-H(57)	120.0
C(58)-C(57)-H(57)	120.0
C(59)-C(58)-C(57)	120.0
C(59)-C(58)-H(58)	120.0
C(57)-C(58)-H(58)	120.0
C(60)-C(59)-C(58)	120.0
C(60)-C(59)-H(59)	120.0
C(58)-C(59)-H(59)	120.0
C(61)-C(60)-C(59)	120.0
C(61)-C(60)-H(60)	120.0
C(59)-C(60)-H(60)	120.0
C(60)-C(61)-C(56)	120.0
C(60)-C(61)-H(61)	120.0
C(56)-C(61)-H(61)	120.0

Table 7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for g39jas. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

Atom	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	32(1)	31(1)	42(2)	2(1)	6(1)	6(1)
C(2)	25(1)	38(2)	48(2)	2(1)	1(1)	4(1)
C(3)	22(1)	33(1)	48(2)	0(1)	2(1)	1(1)
C(4)	29(1)	35(2)	31(1)	2(1)	2(1)	-3(1)
C(5)	45(2)	46(2)	35(2)	1(1)	3(1)	6(1)
C(6)	67(2)	79(3)	33(2)	5(2)	12(2)	5(2)
C(7)	77(2)	68(2)	44(2)	27(2)	8(2)	-5(2)
C(8)	65(2)	44(2)	50(2)	16(2)	1(2)	1(2)
C(9)	45(2)	35(2)	39(2)	6(1)	3(1)	1(1)
C(10)	36(1)	27(1)	31(1)	0(1)	0(1)	4(1)
C(11)	38(2)	32(1)	35(2)	2(1)	0(1)	3(1)

C(12)	47(2)	37(2)	44(2)	-4(1)	-12(1)	-1(1)
C(13)	79(2)	47(2)	34(2)	-11(1)	-1(2)	8(2)
C(14)	82(2)	60(2)	36(2)	-7(2)	19(2)	-2(2)
C(15)	56(2)	43(2)	39(2)	2(1)	9(1)	-8(1)
C(16)	31(1)	28(1)	37(2)	1(1)	-2(1)	-4(1)
C(17)	34(2)	49(2)	39(2)	4(1)	2(1)	6(1)
C(18)	52(2)	60(2)	44(2)	2(2)	12(2)	12(2)
C(19)	70(2)	57(2)	37(2)	-6(2)	5(2)	1(2)
C(20)	56(2)	100(3)	48(2)	-18(2)	-16(2)	5(2)
C(21)	37(2)	91(3)	52(2)	-16(2)	-6(2)	7(2)
C(22)	29(1)	26(1)	40(2)	-3(1)	9(1)	2(1)
C(23)	34(1)	33(2)	42(2)	-1(1)	10(1)	3(1)
C(24)	51(2)	35(2)	50(2)	6(1)	14(1)	12(1)
C(25)	59(2)	29(2)	75(2)	6(2)	32(2)	5(1)
C(26)	41(2)	34(2)	100(3)	5(2)	14(2)	-10(1)
C(27)	37(2)	36(2)	70(2)	2(2)	-3(2)	-4(1)
C(28)	22(1)	36(2)	43(2)	-2(1)	-4(1)	3(1)
C(29)	43(2)	32(2)	58(2)	-3(1)	6(1)	1(1)
C(30)	49(2)	47(2)	48(2)	-11(1)	11(2)	2(1)
C(31)	32(2)	54(2)	41(2)	-1(1)	-1(1)	0(1)
C(32)	49(2)	40(2)	50(2)	5(1)	3(1)	4(1)
C(33)	48(2)	36(2)	42(2)	-1(1)	1(1)	5(1)
C(34)	80(3)	84(3)	56(2)	22(2)	23(2)	4(2)
C(35)	30(1)	51(2)	41(2)	-1(1)	2(1)	3(1)
C(36)	42(2)	41(2)	73(2)	14(2)	6(2)	5(1)
C(37)	24(1)	23(1)	41(2)	-3(1)	1(1)	3(1)
C(38)	33(2)	32(2)	49(2)	-1(1)	8(1)	1(1)
C(39)	36(2)	33(2)	73(2)	0(2)	16(2)	-8(1)
C(40)	33(2)	41(2)	77(2)	-15(2)	-2(2)	-8(1)
C(41)	36(2)	49(2)	51(2)	-10(2)	-10(1)	7(1)
C(42)	28(1)	37(2)	44(2)	-3(1)	0(1)	4(1)
C(43)	45(2)	62(2)	39(2)	10(2)	-2(1)	8(2)
O(1)	22(1)	31(1)	49(1)	1(1)	2(1)	2(1)
O(2)	66(2)	72(2)	45(1)	-2(1)	14(1)	-4(1)
P(1)	28(1)	26(1)	30(1)	0(1)	3(1)	0(1)
P(2)	22(1)	27(1)	39(1)	-1(1)	1(1)	-1(1)

Pd(1)	21(1)	26(1)	34(1)	0(1)	2(1)	-1(1)
Si(1)	23(1)	30(1)	42(1)	2(1)	1(1)	1(1)
C(44)	73(4)	66(5)	59(4)	9(4)	-4(4)	-2(4)
C(45)	57(4)	71(4)	53(4)	1(4)	0(3)	11(4)
C(46)	58(4)	71(4)	58(4)	11(4)	-4(4)	12(4)
C(47)	72(4)	74(5)	58(5)	11(4)	-12(4)	-6(4)
C(48)	89(5)	79(5)	67(4)	18(4)	-15(4)	-12(5)
C(49)	84(5)	74(4)	70(4)	18(4)	-8(5)	-8(4)
C(50)	26(4)	19(5)	35(4)	-2(4)	-6(3)	11(4)
C(51)	29(5)	26(6)	46(4)	10(4)	1(3)	16(3)
C(52)	32(5)	30(6)	45(4)	-3(4)	1(3)	19(4)
C(53)	40(5)	28(6)	33(4)	2(4)	1(4)	14(4)
C(54)	23(4)	29(6)	39(3)	9(4)	-12(3)	13(4)
C(55)	30(5)	21(5)	46(4)	1(4)	3(3)	20(4)
C(56)	70(3)	63(3)	65(3)	-2(3)	-10(3)	6(3)
C(57)	59(3)	74(3)	53(3)	-3(3)	1(3)	13(3)
C(58)	59(3)	73(4)	54(3)	7(3)	-13(3)	21(3)
C(59)	79(3)	63(3)	51(4)	7(3)	-15(3)	10(3)
C(60)	85(4)	70(3)	64(4)	16(3)	-21(3)	-10(4)
C(61)	95(5)	68(4)	75(3)	15(3)	-21(4)	-7(4)

Table 8. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for g39jas.

Atom	x	y	z	U(eq)
H(1A)	5484	2225	2120	41
H(1B)	5516	3369	1675	41
H(2A)	5416	3788	3026	45
H(2B)	6795	3683	2755	45
H(3A)	6292	5378	2087	42
H(3B)	6635	5751	2840	42
H(5)	2542	3406	3239	50

H(6)	2264	2233	4125	72
H(7)	2598	151	4066	75
H(8)	3259	-763	3143	64
H(9)	3588	399	2271	48
H(11)	1372	970	1549	42
H(12)	748	-195	569	54
H(13)	1913	114	-301	65
H(14)	3739	1563	-205	72
H(15)	4390	2732	765	56
H(17)	2397	6660	3215	49
H(18)	2182	7400	4258	61
H(19)	3964	7606	5047	67
H(20)	5974	7044	4787	85
H(21)	6209	6346	3739	74
H(23)	3149	7328	1531	43
H(24)	3759	9048	973	53
H(25)	5805	10150	1237	62
H(26)	7216	9612	2091	71
H(27)	6620	7900	2659	59
H(29)	-394	8536	3247	54
H(30)	-1041	8293	4259	58
H(32)	-1090	4594	3977	56
H(33)	-453	4846	2964	51
H(34A)	-2674	4813	4716	108
H(34B)	-2270	5312	5452	108
H(34C)	-1233	4686	5056	108
H(35A)	-963	6096	1121	61
H(35B)	-1979	6537	1591	61
H(35C)	-1415	5226	1664	61
H(36A)	958	8980	2310	78
H(36B)	-520	8831	1969	78
H(36C)	660	8608	1553	78
H(38)	280	2975	2508	45
H(39)	-1730	1926	2058	57
H(40)	-2385	1964	964	63
H(41)	-1062	3020	311	56

H(43A)	1242	5272	694	73
H(43B)	882	4178	139	73
H(43C)	2140	4156	655	73
H(44)	32	8266	5458	80
H(45)	1464	9393	4861	73
H(46)	3547	10203	5343	75
H(47)	4199	9886	6422	84
H(48)	2767	8758	7019	97
H(49)	684	7948	6537	93
H(50)	5764	6135	954	32
H(51)	7033	4576	650	39
H(52)	6359	3299	-291	42
H(53)	4416	3582	-926	40
H(54)	3147	5141	-622	37
H(55)	3821	6418	318	38
H(56)	374	7795	5638	81
H(57)	988	9294	4939	74
H(58)	2962	10568	5187	75
H(59)	4321	10342	6134	79
H(60)	3707	8843	6833	91
H(61)	1733	7570	6585	98

X-Ray Crystal Structure of 7z (ga49qas)

Crystal Data and Structure Refinement for ga49qas:

Identification code	ga49qas	
Empirical formula	C46 H44 O2 P2 Pd Si	
Formula weight	825.24	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.7826(7) Å b = 17.1122(11) Å c = 12.4527(8) Å	α= 90°. β= 115.206(4)°. γ = 90°.
Volume	2078.9(2) Å ³	
Z	2	
Density (calculated)	1.318 Mg/m ³	
Absorption coefficient	0.588 mm ⁻¹	
F(000)	852	
Crystal size	0.42 x 0.21 x 0.10 mm ³	
Theta range for data collection	1.81 to 27.48°.	
Index ranges	-13<=h<=13, -22<=k<=22, -16<=l<=16	
Reflections collected	23872	
Independent reflections	9098 [R(int) = 0.0289]	
Completeness to theta = 27.48°	99.5 %	
Absorption correction	Integration	
Max. and min. transmission	0.9466 and 0.7971	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9098 / 72 / 493	
Goodness-of-fit on F ²	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0646	
R indices (all data)	R1 = 0.0330, wR2 = 0.0667	
Absolute structure parameter	-0.014(15)	
Largest diff. peak and hole	0.666 and -0.242 e.Å ⁻³	

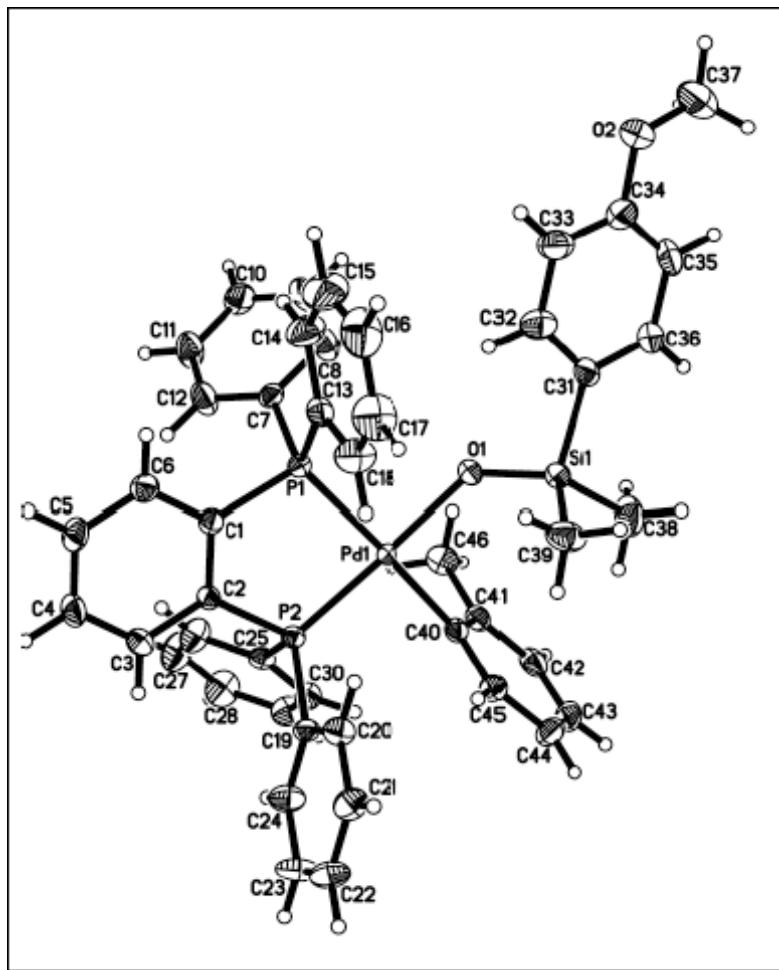


Figure 3. X-ray crystal structure of complex **7z**.

The crystals were obtained directly from recrystallization as yellow needles $0.36 \times 0.26 \times 0.08$ mm in size and mounted using oil (Paratone-N, Exxon) to a 0.3 mm cryo-loop (Hampton Research) with the (-7 -6 -2) scattering planes roughly normal to the spindle axis. Systematic absences for **7z** were consistent with the space group $P\bar{1}$. Unit cell dimensions were $a = 10.7826(7)$ Å, $b = 17.1122(11)$ Å, $c = 12.4527(8)$ Å, $\alpha = 90^\circ$, $\beta = 115.206(4)^\circ$, $\gamma = 90^\circ$. Integration absorption correction was applied (absorption coefficient $\mu = 0.588$ mm⁻¹), and maximum and minimum transmission factors were 0.9466 and 0.7971. The 9098 data points were used in the full-matrix least-squares refinement. The structure

was solved using direct methods by using SHELXTL software package. Hydrogen atoms were placed in “idealized” positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga49qas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	1393(3)	2546(2)	4503(2)	26(1)
C(2)	490(3)	1944(2)	4429(2)	25(1)
C(3)	-888(3)	2008(2)	3624(3)	35(1)
C(4)	-1335(3)	2661(2)	2899(3)	40(1)
C(5)	-439(3)	3259(2)	2985(3)	39(1)
C(6)	918(3)	3206(2)	3781(3)	34(1)
C(7)	4080(3)	2284(2)	4609(2)	29(1)
C(8)	5490(3)	2237(2)	5160(3)	54(1)
C(9)	6215(3)	2089(3)	4485(3)	61(1)
C(10)	5539(4)	1976(2)	3283(3)	51(1)
C(11)	4151(4)	1997(2)	2752(3)	57(1)
C(12)	3417(3)	2160(2)	3412(3)	50(1)
C(13)	3688(3)	3363(2)	6239(2)	33(1)
C(14)	4484(4)	3891(2)	5978(3)	56(1)
C(15)	4815(5)	4601(2)	6590(4)	74(1)
C(16)	4397(5)	4776(2)	7447(4)	74(1)
C(17)	3599(5)	4254(2)	7702(4)	69(1)
C(18)	3244(4)	3546(2)	7112(3)	54(1)
C(19)	-116(3)	1038(2)	6061(2)	27(1)
C(20)	-11(3)	1592(2)	6919(3)	35(1)
C(21)	-936(3)	1587(2)	7428(3)	42(1)
C(22)	-1948(4)	1023(2)	7098(3)	50(1)
C(23)	-2048(4)	483(2)	6263(4)	55(1)
C(24)	-1136(3)	477(2)	5736(3)	43(1)
C(25)	801(3)	261(2)	4458(2)	28(1)

C(26)	400(4)	338(2)	3243(3)	47(1)
C(27)	180(4)	-322(2)	2543(3)	59(1)
C(28)	361(4)	-1054(2)	3039(3)	57(1)
C(29)	771(4)	-1140(2)	4242(3)	44(1)
C(30)	987(3)	-481(2)	4939(3)	35(1)
C(31)	7559(3)	2244(2)	9502(2)	36(1)
C(32)	7368(4)	2972(2)	8939(3)	46(1)
C(33)	8432(4)	3491(2)	9142(3)	51(1)
C(34)	9725(4)	3281(2)	9911(3)	53(1)
C(35)	9994(4)	2581(3)	10466(3)	59(1)
C(36)	8883(4)	2051(2)	10255(3)	53(1)
C(37)	12101(5)	3570(6)	10723(9)	88(2)
C(38)	6684(4)	656(2)	9990(3)	64(1)
C(39)	4900(4)	2052(2)	9772(3)	55(1)
C(40)	3295(3)	320(2)	7583(2)	27(1)
C(41)	4033(3)	-333(2)	7513(2)	33(1)
C(42)	4192(3)	-965(2)	8268(3)	41(1)
C(43)	3672(4)	-945(2)	9098(3)	47(1)
C(44)	2935(3)	-313(2)	9170(3)	43(1)
C(45)	2749(3)	315(2)	8419(2)	34(1)
C(46)	4644(3)	-364(2)	6624(3)	46(1)
O(1)	5293(2)	1505(1)	7747(2)	32(1)
O(2)	10715(6)	3857(5)	10107(7)	76(2)
Si(1)	6026(1)	1587(1)	9149(1)	31(1)
Pd(1)	3271(1)	1316(1)	6659(1)	22(1)
P(1)	3172(1)	2415(1)	5539(1)	25(1)
P(2)	1121(1)	1105(1)	5424(1)	24(1)
O(3)	10760(20)	3750(18)	9883(14)	75(4)
C(47)	11800(20)	3941(18)	11047(15)	73(4)

Table 10. Bond lengths [\AA] and angles [$^\circ$] for ga49qas.

C(1)-C(2)	1.394(4)
C(1)-C(6)	1.397(4)
C(1)-P(1)	1.812(3)
C(2)-C(3)	1.398(4)
C(2)-P(2)	1.828(3)
C(3)-C(4)	1.387(4)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.380(4)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.377(4)
C(5)-H(5A)	0.9500
C(6)-H(6A)	0.9500
C(7)-C(12)	1.368(4)
C(7)-C(8)	1.378(4)
C(7)-P(1)	1.820(3)
C(8)-C(9)	1.393(4)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.371(5)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.355(5)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.390(4)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-C(14)	1.377(4)
C(13)-C(18)	1.397(4)
C(13)-P(1)	1.814(3)
C(14)-C(15)	1.398(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.356(6)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.368(6)
C(16)-H(30o)	0.9500
C(17)-C(18)	1.384(5)

C(17)-H(31o)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(24)	1.384(4)
C(19)-C(20)	1.397(4)
C(19)-P(2)	1.824(2)
C(20)-C(21)	1.390(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.381(4)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.361(5)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.396(4)
C(23)-H(23A)	0.9500
C(24)-H(24A)	0.9500
C(25)-C(30)	1.381(4)
C(25)-C(26)	1.392(4)
C(25)-P(2)	1.816(3)
C(26)-C(27)	1.384(5)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.373(5)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.377(5)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.382(4)
C(29)-H(29A)	0.9500
C(30)-H(30A)	0.9500
C(31)-C(36)	1.373(5)
C(31)-C(32)	1.402(5)
C(31)-Si(1)	1.889(3)
C(32)-C(33)	1.386(5)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.361(5)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.352(5)
C(34)-O(3)	1.384(10)
C(34)-O(2)	1.395(5)

C(35)-C(36)	1.434(5)
C(35)-H(35A)	0.9500
C(36)-H(36A)	0.9500
C(37)-O(2)	1.445(7)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-Si(1)	1.872(4)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-Si(1)	1.875(3)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(41)	1.396(4)
C(40)-C(45)	1.396(4)
C(40)-Pd(1)	2.051(3)
C(41)-C(42)	1.394(4)
C(41)-C(46)	1.512(4)
C(42)-C(43)	1.371(4)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.369(5)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.382(4)
C(44)-H(44A)	0.9500
C(45)-H(45A)	0.9500
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
O(1)-Si(1)	1.5860(19)
O(1)-Pd(1)	2.0440(18)
Pd(1)-P(2)	2.1985(7)
Pd(1)-P(1)	2.3161(7)
O(3)-C(47)	1.444(9)
C(47)-H(47A)	0.9800

C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(2)-C(1)-C(6)	120.0(3)
C(2)-C(1)-P(1)	116.9(2)
C(6)-C(1)-P(1)	123.1(2)
C(1)-C(2)-C(3)	119.3(2)
C(1)-C(2)-P(2)	119.2(2)
C(3)-C(2)-P(2)	121.5(2)
C(4)-C(3)-C(2)	119.9(3)
C(4)-C(3)-H(3A)	120.1
C(2)-C(3)-H(3A)	120.1
C(5)-C(4)-C(3)	120.6(3)
C(5)-C(4)-H(4A)	119.7
C(3)-C(4)-H(4A)	119.7
C(6)-C(5)-C(4)	120.1(3)
C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(6)-C(1)	120.2(3)
C(5)-C(6)-H(6A)	119.9
C(1)-C(6)-H(6A)	119.9
C(12)-C(7)-C(8)	119.1(3)
C(12)-C(7)-P(1)	122.6(2)
C(8)-C(7)-P(1)	118.0(2)
C(7)-C(8)-C(9)	119.6(3)
C(7)-C(8)-H(8A)	120.2
C(9)-C(8)-H(8A)	120.2
C(10)-C(9)-C(8)	120.7(3)
C(10)-C(9)-H(9A)	119.7
C(8)-C(9)-H(9A)	119.7
C(11)-C(10)-C(9)	119.5(3)
C(11)-C(10)-H(10A)	120.3
C(9)-C(10)-H(10A)	120.3
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11A)	119.8
C(12)-C(11)-H(11A)	119.8

C(7)-C(12)-C(11)	120.7(3)
C(7)-C(12)-H(12A)	119.7
C(11)-C(12)-H(12A)	119.7
C(14)-C(13)-C(18)	119.4(3)
C(14)-C(13)-P(1)	124.6(2)
C(18)-C(13)-P(1)	116.0(2)
C(13)-C(14)-C(15)	118.8(3)
C(13)-C(14)-H(14A)	120.6
C(15)-C(14)-H(14A)	120.6
C(16)-C(15)-C(14)	121.8(4)
C(16)-C(15)-H(15A)	119.1
C(14)-C(15)-H(15A)	119.1
C(15)-C(16)-C(17)	119.4(4)
C(15)-C(16)-H(30o)	120.3
C(17)-C(16)-H(30o)	120.3
C(16)-C(17)-C(18)	120.5(4)
C(16)-C(17)-H(31o)	119.7
C(18)-C(17)-H(31o)	119.7
C(17)-C(18)-C(13)	120.0(3)
C(17)-C(18)-H(18A)	120.0
C(13)-C(18)-H(18A)	120.0
C(24)-C(19)-C(20)	119.4(2)
C(24)-C(19)-P(2)	123.6(2)
C(20)-C(19)-P(2)	117.0(2)
C(21)-C(20)-C(19)	120.2(3)
C(21)-C(20)-H(20A)	119.9
C(19)-C(20)-H(20A)	119.9
C(22)-C(21)-C(20)	119.9(3)
C(22)-C(21)-H(21A)	120.0
C(20)-C(21)-H(21A)	120.0
C(23)-C(22)-C(21)	119.8(3)
C(23)-C(22)-H(22A)	120.1
C(21)-C(22)-H(22A)	120.1
C(22)-C(23)-C(24)	121.4(3)
C(22)-C(23)-H(23A)	119.3
C(24)-C(23)-H(23A)	119.3

C(19)-C(24)-C(23)	119.2(3)
C(19)-C(24)-H(24A)	120.4
C(23)-C(24)-H(24A)	120.4
C(30)-C(25)-C(26)	118.6(3)
C(30)-C(25)-P(2)	119.5(2)
C(26)-C(25)-P(2)	121.9(2)
C(27)-C(26)-C(25)	119.9(3)
C(27)-C(26)-H(26A)	120.1
C(25)-C(26)-H(26A)	120.1
C(28)-C(27)-C(26)	120.5(3)
C(28)-C(27)-H(27A)	119.8
C(26)-C(27)-H(27A)	119.8
C(27)-C(28)-C(29)	120.4(3)
C(27)-C(28)-H(28A)	119.8
C(29)-C(28)-H(28A)	119.8
C(28)-C(29)-C(30)	119.1(3)
C(28)-C(29)-H(29A)	120.5
C(30)-C(29)-H(29A)	120.5
C(25)-C(30)-C(29)	121.5(3)
C(25)-C(30)-H(30A)	119.2
C(29)-C(30)-H(30A)	119.2
C(36)-C(31)-C(32)	116.3(3)
C(36)-C(31)-Si(1)	124.6(3)
C(32)-C(31)-Si(1)	119.0(2)
C(33)-C(32)-C(31)	123.0(4)
C(33)-C(32)-H(32A)	118.5
C(31)-C(32)-H(32A)	118.5
C(34)-C(33)-C(32)	118.6(4)
C(34)-C(33)-H(33A)	120.7
C(32)-C(33)-H(33A)	120.7
C(35)-C(34)-C(33)	121.7(3)
C(35)-C(34)-O(3)	121.8(13)
C(33)-C(34)-O(3)	115.0(11)
C(35)-C(34)-O(2)	123.7(5)
C(33)-C(34)-O(2)	114.5(5)
C(34)-C(35)-C(36)	119.1(3)

C(34)-C(35)-H(35A)	120.5
C(36)-C(35)-H(35A)	120.5
C(31)-C(36)-C(35)	121.2(3)
C(31)-C(36)-H(36A)	119.4
C(35)-C(36)-H(36A)	119.4
Si(1)-C(38)-H(38A)	109.5
Si(1)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
Si(1)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
Si(1)-C(39)-H(39A)	109.5
Si(1)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
Si(1)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(45)	118.3(2)
C(41)-C(40)-Pd(1)	120.09(19)
C(45)-C(40)-Pd(1)	121.0(2)
C(42)-C(41)-C(40)	119.2(3)
C(42)-C(41)-C(46)	120.0(3)
C(40)-C(41)-C(46)	120.8(3)
C(43)-C(42)-C(41)	121.1(3)
C(43)-C(42)-H(42A)	119.4
C(41)-C(42)-H(42A)	119.4
C(44)-C(43)-C(42)	120.3(3)
C(44)-C(43)-H(43A)	119.9
C(42)-C(43)-H(43A)	119.9
C(43)-C(44)-C(45)	119.5(3)
C(43)-C(44)-H(44A)	120.3
C(45)-C(44)-H(44A)	120.3
C(44)-C(45)-C(40)	121.5(3)
C(44)-C(45)-H(45A)	119.2
C(40)-C(45)-H(45A)	119.2
C(41)-C(46)-H(46A)	109.5

C(41)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(41)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
Si(1)-O(1)-Pd(1)	129.39(10)
C(34)-O(2)-C(37)	113.2(7)
O(1)-Si(1)-C(38)	115.66(14)
O(1)-Si(1)-C(39)	112.69(14)
C(38)-Si(1)-C(39)	106.7(2)
O(1)-Si(1)-C(31)	106.59(11)
C(38)-Si(1)-C(31)	106.90(17)
C(39)-Si(1)-C(31)	107.90(14)
O(1)-Pd(1)-C(40)	90.25(9)
O(1)-Pd(1)-P(2)	177.47(5)
C(40)-Pd(1)-P(2)	90.77(8)
O(1)-Pd(1)-P(1)	91.92(5)
C(40)-Pd(1)-P(1)	177.41(8)
P(2)-Pd(1)-P(1)	87.00(2)
C(1)-P(1)-C(13)	104.24(13)
C(1)-P(1)-C(7)	104.80(12)
C(13)-P(1)-C(7)	106.15(13)
C(1)-P(1)-Pd(1)	107.03(9)
C(13)-P(1)-Pd(1)	120.68(9)
C(7)-P(1)-Pd(1)	112.56(9)
C(25)-P(2)-C(19)	105.70(12)
C(25)-P(2)-C(2)	105.39(12)
C(19)-P(2)-C(2)	102.35(11)
C(25)-P(2)-Pd(1)	116.15(9)
C(19)-P(2)-Pd(1)	117.03(9)
C(2)-P(2)-Pd(1)	108.78(9)
C(34)-O(3)-C(47)	113.5(10)
O(3)-C(47)-H(47A)	109.5
O(3)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
O(3)-C(47)-H(47C)	109.5

H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5

Table 11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga49qas. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	26(1)	28(1)	26(1)	1(1)	13(1)	3(1)
C(2)	21(1)	29(1)	26(1)	2(1)	11(1)	4(1)
C(3)	26(2)	40(2)	38(2)	2(1)	13(1)	3(1)
C(4)	30(2)	46(2)	38(2)	9(1)	8(1)	12(1)
C(5)	41(2)	33(2)	40(2)	12(1)	14(1)	14(1)
C(6)	34(2)	28(1)	39(2)	5(1)	16(1)	3(1)
C(7)	30(1)	28(1)	32(1)	8(1)	15(1)	3(1)
C(8)	30(2)	93(3)	36(2)	-4(2)	12(1)	7(2)
C(9)	27(2)	104(3)	55(2)	-5(2)	20(2)	5(2)
C(10)	45(2)	67(2)	52(2)	11(2)	32(2)	11(2)
C(11)	42(2)	98(3)	31(2)	0(2)	16(2)	11(2)
C(12)	29(2)	86(3)	32(2)	0(2)	11(1)	7(2)
C(13)	34(2)	26(1)	33(1)	-1(1)	7(1)	-2(1)
C(14)	76(3)	43(2)	53(2)	-3(2)	31(2)	-21(2)
C(15)	101(4)	42(2)	76(3)	-6(2)	34(3)	-31(2)
C(16)	97(4)	42(2)	61(2)	-17(2)	12(2)	-8(2)
C(17)	88(3)	54(2)	70(3)	-28(2)	37(3)	-6(2)
C(18)	64(2)	51(2)	56(2)	-16(2)	35(2)	-10(2)
C(19)	24(1)	30(1)	32(1)	2(1)	15(1)	0(1)
C(20)	36(2)	35(2)	39(2)	-7(1)	20(1)	-2(1)
C(21)	50(2)	45(2)	41(2)	-5(1)	29(2)	3(1)
C(22)	50(2)	57(2)	62(2)	-2(2)	42(2)	0(2)
C(23)	48(2)	53(2)	83(3)	-15(2)	46(2)	-19(2)
C(24)	44(2)	41(2)	53(2)	-11(1)	30(2)	-8(1)
C(25)	27(2)	29(2)	31(1)	-6(1)	15(1)	-2(1)
C(26)	65(2)	40(2)	38(2)	-2(1)	25(2)	4(2)
C(27)	91(3)	52(2)	35(2)	-9(2)	27(2)	3(2)

C(28)	79(3)	42(2)	52(2)	-19(2)	29(2)	-7(2)
C(29)	54(2)	32(2)	50(2)	-7(1)	25(2)	-5(2)
C(30)	39(2)	30(2)	34(2)	-2(1)	14(1)	-2(1)
C(31)	33(2)	50(2)	25(1)	-10(1)	13(1)	-8(1)
C(32)	48(2)	45(2)	55(2)	-5(2)	31(2)	-6(2)
C(33)	52(2)	50(2)	54(2)	-2(2)	27(2)	-12(2)
C(34)	58(2)	60(2)	39(2)	2(2)	19(2)	-17(2)
C(35)	36(2)	89(3)	34(2)	5(2)	-1(1)	-6(2)
C(36)	44(2)	72(2)	34(2)	5(2)	8(2)	-13(2)
C(37)	55(3)	97(4)	88(4)	12(4)	6(3)	-22(3)
C(38)	66(3)	45(2)	51(2)	12(2)	-2(2)	-8(2)
C(39)	53(2)	65(2)	59(2)	-26(2)	34(2)	-22(2)
C(40)	26(1)	23(1)	27(1)	0(1)	7(1)	-3(1)
C(41)	28(1)	31(2)	35(2)	1(1)	7(1)	-3(1)
C(42)	32(2)	28(2)	50(2)	4(1)	3(1)	-2(1)
C(43)	51(2)	38(2)	43(2)	12(1)	11(2)	-8(2)
C(44)	51(2)	43(2)	34(2)	4(1)	19(2)	-10(2)
C(45)	34(2)	32(2)	33(1)	4(1)	11(1)	-4(1)
C(46)	41(2)	44(2)	55(2)	-3(2)	24(2)	6(2)
O(1)	25(1)	41(1)	28(1)	0(1)	8(1)	-4(1)
O(2)	58(2)	93(4)	59(3)	15(3)	7(2)	-36(2)
Si(1)	30(1)	33(1)	28(1)	-2(1)	10(1)	-6(1)
Pd(1)	22(1)	23(1)	22(1)	1(1)	10(1)	0(1)
P(1)	24(1)	25(1)	25(1)	3(1)	10(1)	-1(1)
P(2)	22(1)	25(1)	25(1)	-1(1)	11(1)	0(1)
O(3)	55(5)	81(5)	70(5)	7(5)	10(4)	-22(4)
C(47)	59(5)	84(6)	62(5)	6(5)	12(4)	-29(5)

Table 12. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga49qas.

Atom	x	y	z	U(eq)
H(3A)	-1516	1604	3572	42
H(4A)	-2267	2697	2340	48
H(5A)	-758	3707	2493	47
H(6A)	1532	3619	3839	40
H(8A)	5964	2304	5994	65
H(9A)	7188	2067	4862	73
H(10A)	6040	1883	2826	61
H(11A)	3677	1900	1924	68
H(12A)	2445	2185	3027	60
H(14A)	4803	3774	5393	68
H(15A)	5347	4972	6400	89
H(30o)	4656	5257	7866	89
H(31o)	3287	4379	8288	83
H(18A)	2698	3184	7301	64
H(20A)	695	1974	7156	42
H(21A)	-872	1970	8001	50
H(22A)	-2572	1013	7453	60
H(23A)	-2755	101	6034	66
H(24A)	-1214	92	5160	51
H(26A)	277	843	2895	56
H(27A)	-99	-268	1713	71
H(28A)	203	-1503	2550	69
H(29A)	904	-1646	4587	53
H(30A)	1270	-539	5769	41
H(32A)	6469	3117	8393	56
H(33A)	8262	3983	8752	61
H(35A)	10906	2441	10989	70
H(36A)	9066	1558	10644	63
H(37A)	12748	3996	10819	133
H(37B)	12253	3146	10263	133

H(37C)	12243	3373	11506	133
H(38A)	7286	394	9695	95
H(38B)	5910	313	9878	95
H(38C)	7199	773	10836	95
H(39A)	4155	1694	9685	83
H(39B)	4513	2538	9342	83
H(39C)	5442	2169	10615	83
H(42A)	4670	-1416	8205	50
H(43A)	3823	-1373	9625	56
H(44A)	2555	-305	9732	51
H(45A)	2237	754	8472	41
H(46A)	5087	-871	6677	69
H(46B)	5324	54	6795	69
H(46C)	3916	-294	5821	69
H(47A)	12608	4150	10973	109
H(47B)	12058	3470	11540	109
H(47C)	11446	4334	11416	109

X-Ray data for 7t (ga71pas)**Crystal data and structure refinement for ga71pas:**

Identification code	ga71pas
Empirical formula	C52 H50 O2 P2 Pd Si
Formula weight	903.35
Temperature	193(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 12.5239(3) Å $\alpha = 90.909(2)^\circ$. b = 12.6398(4) Å $\beta = 105.1700(10)^\circ$. c = 15.2157(4) Å $\gamma = 103.595(2)^\circ$.
Volume	2251.87(11) Å ³
Z	2
Density (calculated)	1.332 Mg/m ³
Absorption coefficient	0.549 mm ⁻¹
F(000)	936
Crystal size	0.40 x 0.30 x 0.04 mm ³
Theta range for data collection	1.74 to 27.91°.
Index ranges	-16<=h<=16, -16<=k<=16, -20<=l<=20
Reflections collected	36554
Independent reflections	10754 [R(int) = 0.0425]
Completeness to theta = 27.91°	99.7 %
Absorption correction	Integration
Max. and min. transmission	0.9786 and 0.8679
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10754 / 258 / 577
Goodness-of-fit on F ²	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0778
R indices (all data)	R1 = 0.0522, wR2 = 0.0847
Largest diff. peak and hole	1.069 and -0.340 e.Å ⁻³

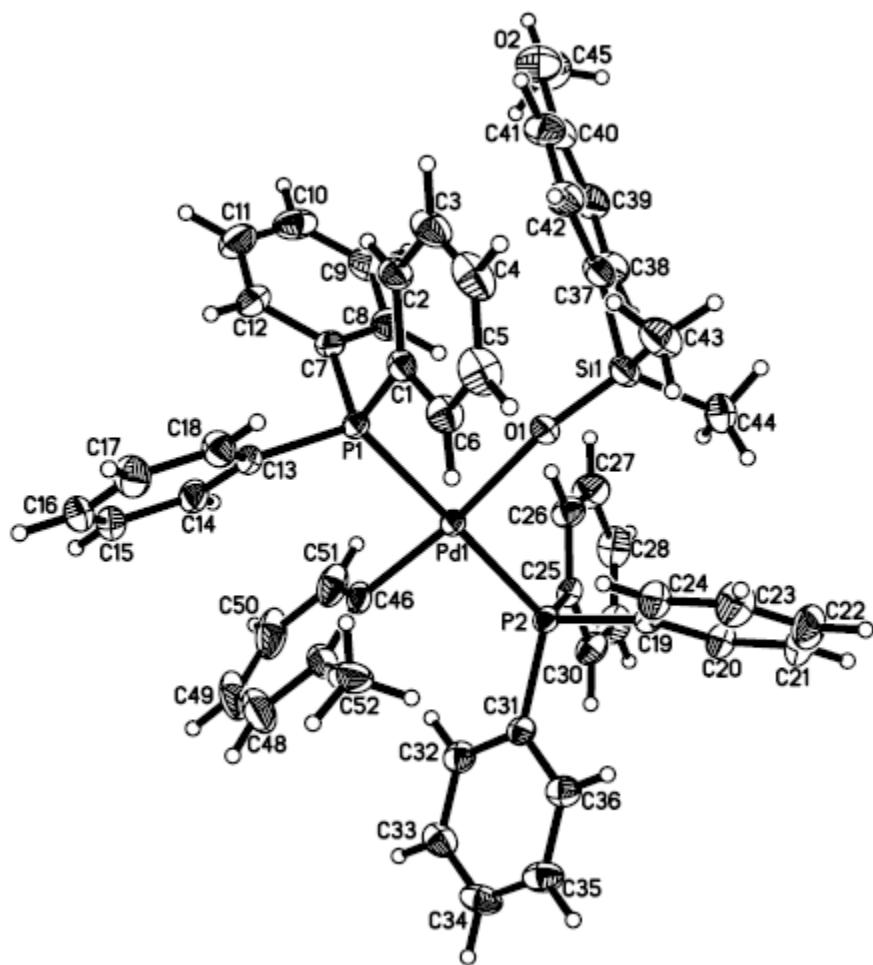


Figure 4. X-ray structure of complex **7t**.

The crystals were obtained directly from recrystallization as yellow needles 0.40 x 0.30 x 0.04 mm in size and mounted using oil (Parantone-N, Exxon) to a thin glass fiber with the (1 0 0) scattering planes roughly normal to the spindle axis. Systematic absences for **7t** were consistent with the space group P-1. Unit cell dimensions were $a = 12.5239(3)$ Å, $b = 12.6398(4)$ Å, $c = 15.2157(11)$ Å, $\alpha = 90.909(2)^\circ$, $\beta = 105.1700(10)^\circ$, $\gamma = 103.595(2)^\circ$. Integration absorption correction was applied (absorption coefficient $\mu = 0.549$ mm⁻¹), and maximum and minimum transmission factors were 0.9786 and 0.8679. The 10754 data points were used in the full-matrix

least-squares refinement. The structure was solved using direct methods by using SHELXTL software package. Hydrogen atoms were placed in “idealized” positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 13. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga71pas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Pd(1)	9746(1)	3941(1)	2363(1)	26(1)
P(1)	7844(1)	3996(1)	1914(1)	28(1)
P(2)	11650(1)	3906(1)	2778(1)	27(1)
Si(1)	8974(1)	993(1)	2292(1)	41(1)
O(1)	9223(12)	2268(2)	2390(6)	40(2)
O(2)	5775(2)	-660(2)	4648(2)	67(1)
C(1)	7043(2)	2951(2)	985(2)	33(1)
C(2)	5984(2)	2271(2)	963(2)	41(1)
C(3)	5405(2)	1519(2)	216(2)	54(1)
C(4)	5864(3)	1446(2)	-497(2)	58(1)
C(5)	6907(3)	2115(3)	-482(2)	57(1)
C(6)	7506(2)	2850(2)	265(2)	44(1)
C(7)	7137(2)	3698(2)	2816(2)	32(1)
C(8)	7523(2)	3046(2)	3485(2)	42(1)
C(9)	6961(3)	2780(3)	4159(2)	55(1)
C(10)	6028(3)	3187(3)	4165(2)	57(1)
C(11)	5645(2)	3828(3)	3503(2)	58(1)
C(12)	6188(2)	4087(2)	2832(2)	48(1)
C(13)	7433(2)	5230(2)	1492(2)	32(1)
C(14)	7779(2)	6172(2)	2081(2)	39(1)
C(15)	7477(2)	7122(2)	1786(2)	43(1)
C(16)	6821(2)	7134(2)	910(2)	48(1)
C(17)	6466(2)	6205(2)	323(2)	50(1)
C(18)	6767(2)	5251(2)	605(2)	41(1)
C(19)	11919(2)	2821(2)	2129(2)	30(1)

C(20)	12808(2)	2332(2)	2484(2)	39(1)
C(21)	13026(2)	1552(2)	1956(2)	51(1)
C(22)	12357(3)	1243(3)	1073(2)	58(1)
C(23)	11471(3)	1719(3)	718(2)	56(1)
C(24)	11246(2)	2502(2)	1240(2)	42(1)
C(25)	12099(2)	3600(2)	3968(2)	30(1)
C(26)	11292(2)	2948(2)	4328(2)	42(1)
C(27)	11608(3)	2615(3)	5205(2)	54(1)
C(28)	12733(3)	2937(3)	5719(2)	52(1)
C(29)	13534(2)	3602(2)	5376(2)	49(1)
C(30)	13221(2)	3943(2)	4507(2)	40(1)
C(31)	12767(2)	5090(2)	2675(2)	31(1)
C(32)	13023(2)	6039(2)	3244(2)	40(1)
C(33)	13860(2)	6945(2)	3167(2)	45(1)
C(34)	14444(2)	6907(2)	2526(2)	49(1)
C(35)	14198(2)	5981(2)	1948(2)	48(1)
C(36)	13359(2)	5076(2)	2021(2)	39(1)
C(37)	7991(2)	457(2)	3026(2)	42(1)
C(38)	8410(2)	358(2)	3959(2)	51(1)
C(39)	7716(3)	3(2)	4527(2)	53(1)
C(40)	6548(3)	-279(2)	4162(2)	50(1)
C(41)	6088(2)	-192(2)	3242(2)	53(1)
C(42)	6800(2)	167(2)	2694(2)	47(1)
C(43)	8266(3)	316(2)	1114(2)	60(1)
C(44)	10260(3)	432(2)	2753(2)	61(1)
C(45)	6226(3)	-686(3)	5606(2)	81(1)
C(46)	10222(3)	5549(2)	2697(2)	37(1)
C(47)	10440(3)	6322(3)	2085(2)	51(1)
C(48)	10788(4)	7427(2)	2378(3)	81(2)
C(49)	10919(4)	7759(2)	3283(3)	86(2)
C(50)	10701(3)	6987(3)	3896(2)	75(2)
C(51)	10353(4)	5882(3)	3603(2)	55(2)
C(52)	10294(6)	5982(5)	1111(4)	65(2)
C(53)	10227(6)	5570(2)	2318(4)	38(2)
C(54)	10438(5)	6234(4)	3113(4)	47(2)
C(55)	10773(7)	7362(4)	3107(4)	69(2)

C(56)	10896(6)	7827(2)	2306(5)	75(2)
C(57)	10684(6)	7164(4)	1512(4)	63(2)
C(58)	10350(6)	6035(4)	1518(4)	46(2)
C(59)	10291(11)	5820(9)	3972(6)	65(2)
O(3)	9280(20)	2250(2)	2167(9)	43(3)

Table 14. Bond lengths [Å] and angles [°] for ga71pas.

Pd(1)-C(46)	1.995(2)
Pd(1)-C(53)	2.012(3)
Pd(1)-O(1)	2.067(2)
Pd(1)-O(3)	2.074(3)
Pd(1)-P(2)	2.3128(6)
Pd(1)-P(1)	2.3186(6)
P(1)-C(7)	1.818(2)
P(1)-C(1)	1.823(2)
P(1)-C(13)	1.830(2)
P(2)-C(19)	1.822(2)
P(2)-C(25)	1.827(2)
P(2)-C(31)	1.832(2)
Si(1)-O(1)	1.564(3)
Si(1)-O(3)	1.571(3)
Si(1)-C(43)	1.870(3)
Si(1)-C(44)	1.885(3)
Si(1)-C(37)	1.891(3)
O(2)-C(40)	1.371(3)
O(2)-C(45)	1.423(4)
C(1)-C(6)	1.384(3)
C(1)-C(2)	1.392(3)
C(2)-C(3)	1.390(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.365(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(4)
C(4)-H(4)	0.9500

C(5)-C(6)	1.383(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(3)
C(7)-C(12)	1.395(3)
C(8)-C(9)	1.392(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.385(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.363(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.371(4)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(3)
C(13)-C(18)	1.393(3)
C(14)-C(15)	1.388(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.373(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.374(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.388(4)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.389(3)
C(19)-C(20)	1.390(3)
C(20)-C(21)	1.382(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.377(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.377(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.382(4)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500

C(25)-C(26)	1.384(3)
C(25)-C(30)	1.391(3)
C(26)-C(27)	1.390(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.380(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.370(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.383(4)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(32)	1.390(3)
C(31)-C(36)	1.390(3)
C(32)-C(33)	1.389(4)
C(32)-H(32)	0.9500
C(33)-C(34)	1.370(4)
C(33)-H(33)	0.9500
C(34)-C(35)	1.376(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.388(4)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.397(4)
C(37)-C(42)	1.399(4)
C(38)-C(39)	1.389(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.377(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.384(4)
C(41)-C(42)	1.381(4)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800

C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-C(47)	1.3900
C(46)-C(51)	1.3900
C(47)-C(48)	1.3900
C(47)-C(52)	1.488(6)
C(48)-C(49)	1.3900
C(48)-H(48)	0.9500
C(49)-C(50)	1.3900
C(49)-H(49)	0.9500
C(50)-C(51)	1.3900
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(54)	1.3900
C(53)-C(58)	1.3900
C(54)-C(55)	1.3900
C(54)-C(59)	1.455(9)
C(55)-C(56)	1.3900
C(55)-H(55)	0.9500
C(56)-C(57)	1.3900
C(56)-H(56)	0.9500
C(57)-C(58)	1.3900
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(46)-Pd(1)-O(1)	163.9(3)
C(53)-Pd(1)-O(1)	178.9(4)
C(46)-Pd(1)-O(3)	173.8(4)

C(53)-Pd(1)-O(3)	169.5(4)
C(46)-Pd(1)-P(2)	88.96(12)
C(53)-Pd(1)-P(2)	89.1(2)
O(1)-Pd(1)-P(2)	91.9(4)
O(3)-Pd(1)-P(2)	89.9(7)
C(46)-Pd(1)-P(1)	90.69(12)
C(53)-Pd(1)-P(1)	90.2(2)
O(1)-Pd(1)-P(1)	88.8(4)
O(3)-Pd(1)-P(1)	90.6(7)
P(2)-Pd(1)-P(1)	178.55(2)
C(7)-P(1)-C(1)	105.14(11)
C(7)-P(1)-C(13)	102.80(10)
C(1)-P(1)-C(13)	103.27(11)
C(7)-P(1)-Pd(1)	112.89(8)
C(1)-P(1)-Pd(1)	110.33(7)
C(13)-P(1)-Pd(1)	120.91(8)
C(19)-P(2)-C(25)	104.56(10)
C(19)-P(2)-C(31)	102.09(10)
C(25)-P(2)-C(31)	104.36(10)
C(19)-P(2)-Pd(1)	112.13(7)
C(25)-P(2)-Pd(1)	110.86(7)
C(31)-P(2)-Pd(1)	121.25(7)
O(1)-Si(1)-C(43)	116.3(3)
O(3)-Si(1)-C(43)	105.3(5)
O(1)-Si(1)-C(44)	114.7(5)
O(3)-Si(1)-C(44)	113.7(9)
C(43)-Si(1)-C(44)	106.38(15)
O(1)-Si(1)-C(37)	107.0(4)
O(3)-Si(1)-C(37)	119.0(8)
C(43)-Si(1)-C(37)	107.18(13)
C(44)-Si(1)-C(37)	104.51(13)
Si(1)-O(1)-Pd(1)	169.3(8)
C(40)-O(2)-C(45)	116.6(3)
C(6)-C(1)-C(2)	119.0(2)
C(6)-C(1)-P(1)	118.06(19)
C(2)-C(1)-P(1)	122.89(19)

C(3)-C(2)-C(1)	119.6(3)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(4)-C(3)-C(2)	120.5(3)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	120.3(3)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	119.9(3)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	120.6(3)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
C(8)-C(7)-C(12)	119.1(2)
C(8)-C(7)-P(1)	119.56(18)
C(12)-C(7)-P(1)	121.31(19)
C(7)-C(8)-C(9)	120.0(3)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	119.8(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(11)-C(10)-C(9)	120.2(3)
C(11)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(7)	120.5(3)
C(11)-C(12)-H(12)	119.7
C(7)-C(12)-H(12)	119.7
C(14)-C(13)-C(18)	118.9(2)
C(14)-C(13)-P(1)	118.88(18)
C(18)-C(13)-P(1)	122.19(19)

C(15)-C(14)-C(13)	120.5(2)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(16)-C(15)-C(14)	120.2(3)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	119.9(2)
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	120.7(3)
C(16)-C(17)-H(17)	119.7
C(18)-C(17)-H(17)	119.7
C(17)-C(18)-C(13)	119.9(2)
C(17)-C(18)-H(18)	120.1
C(13)-C(18)-H(18)	120.1
C(24)-C(19)-C(20)	118.9(2)
C(24)-C(19)-P(2)	119.13(17)
C(20)-C(19)-P(2)	121.90(18)
C(21)-C(20)-C(19)	120.4(2)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	120.3(3)
C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	119.6(3)
C(23)-C(22)-H(22)	120.2
C(21)-C(22)-H(22)	120.2
C(22)-C(23)-C(24)	120.6(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(23)-C(24)-C(19)	120.2(2)
C(23)-C(24)-H(24)	119.9
C(19)-C(24)-H(24)	119.9
C(26)-C(25)-C(30)	118.9(2)
C(26)-C(25)-P(2)	118.01(18)
C(30)-C(25)-P(2)	123.03(18)

C(25)-C(26)-C(27)	120.4(2)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(28)-C(27)-C(26)	119.8(3)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(29)-C(28)-C(27)	120.3(3)
C(29)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	120.0(3)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(25)	120.6(3)
C(29)-C(30)-H(30)	119.7
C(25)-C(30)-H(30)	119.7
C(32)-C(31)-C(36)	118.4(2)
C(32)-C(31)-P(2)	120.15(18)
C(36)-C(31)-P(2)	121.44(18)
C(33)-C(32)-C(31)	120.7(2)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(34)-C(33)-C(32)	119.9(3)
C(34)-C(33)-H(33)	120.1
C(32)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	120.6(3)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	119.7(3)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(35)-C(36)-C(31)	120.8(2)
C(35)-C(36)-H(36)	119.6
C(31)-C(36)-H(36)	119.6
C(38)-C(37)-C(42)	114.9(3)
C(38)-C(37)-Si(1)	121.8(2)
C(42)-C(37)-Si(1)	123.3(2)

C(39)-C(38)-C(37)	123.5(3)
C(39)-C(38)-H(38)	118.2
C(37)-C(38)-H(38)	118.2
C(40)-C(39)-C(38)	119.1(3)
C(40)-C(39)-H(39)	120.5
C(38)-C(39)-H(39)	120.5
O(2)-C(40)-C(39)	124.6(3)
O(2)-C(40)-C(41)	115.7(3)
C(39)-C(40)-C(41)	119.7(3)
C(42)-C(41)-C(40)	120.0(3)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(37)	122.8(3)
C(41)-C(42)-H(42)	118.6
C(37)-C(42)-H(42)	118.6
Si(1)-C(43)-H(43A)	109.5
Si(1)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
Si(1)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
Si(1)-C(44)-H(44A)	109.5
Si(1)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
Si(1)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
O(2)-C(45)-H(45A)	109.5
O(2)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
O(2)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(47)-C(46)-C(51)	120.0
C(47)-C(46)-Pd(1)	123.66(18)
C(51)-C(46)-Pd(1)	116.33(18)

C(48)-C(47)-C(46)	120.0
C(48)-C(47)-C(52)	119.2(3)
C(46)-C(47)-C(52)	120.8(3)
C(47)-C(48)-C(49)	120.0
C(47)-C(48)-H(48)	120.0
C(49)-C(48)-H(48)	120.0
C(50)-C(49)-C(48)	120.0
C(50)-C(49)-H(49)	120.0
C(48)-C(49)-H(49)	120.0
C(49)-C(50)-C(51)	120.0
C(49)-C(50)-H(50)	120.0
C(51)-C(50)-H(50)	120.0
C(50)-C(51)-C(46)	120.0
C(50)-C(51)-H(51)	120.0
C(46)-C(51)-H(51)	120.0
C(54)-C(53)-C(58)	120.0
C(54)-C(53)-Pd(1)	118.4(3)
C(58)-C(53)-Pd(1)	121.6(3)
C(53)-C(54)-C(55)	120.0
C(53)-C(54)-C(59)	123.7(6)
C(55)-C(54)-C(59)	116.3(6)
C(54)-C(55)-C(56)	120.0
C(54)-C(55)-H(55)	120.0
C(56)-C(55)-H(55)	120.0
C(57)-C(56)-C(55)	120.0
C(57)-C(56)-H(56)	120.0
C(55)-C(56)-H(56)	120.0
C(56)-C(57)-C(58)	120.0
C(56)-C(57)-H(57)	120.0
C(58)-C(57)-H(57)	120.0
C(57)-C(58)-C(53)	120.0
C(57)-C(58)-H(58)	120.0
C(53)-C(58)-H(58)	120.0
C(54)-C(59)-H(59A)	109.5
C(54)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5

C(54)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
Si(1)-O(3)-Pd(1)	165.2(9)

Table 15. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga71pas. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12}]$

Atom	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pd(1)	21(1)	25(1)	30(1)	2(1)	4(1)	7(1)
P(1)	22(1)	28(1)	31(1)	2(1)	4(1)	7(1)
P(2)	22(1)	29(1)	28(1)	1(1)	5(1)	7(1)
Si(1)	36(1)	28(1)	53(1)	2(1)	6(1)	5(1)
O(1)	35(2)	28(2)	59(3)	11(2)	16(3)	9(2)
O(2)	63(1)	72(2)	61(1)	10(1)	23(1)	4(1)
C(1)	28(1)	29(1)	36(1)	2(1)	-2(1)	9(1)
C(2)	33(1)	35(1)	48(2)	5(1)	1(1)	5(1)
C(3)	43(2)	36(2)	64(2)	5(1)	-12(1)	1(1)
C(4)	67(2)	41(2)	44(2)	-4(1)	-17(2)	9(2)
C(5)	72(2)	56(2)	36(1)	-3(1)	2(1)	16(2)
C(6)	45(2)	42(2)	39(1)	-1(1)	6(1)	9(1)
C(7)	27(1)	31(1)	36(1)	1(1)	9(1)	4(1)
C(8)	42(1)	43(2)	42(1)	6(1)	14(1)	11(1)
C(9)	61(2)	57(2)	43(2)	11(1)	17(1)	4(2)
C(10)	51(2)	64(2)	55(2)	-10(2)	31(2)	-5(2)
C(11)	43(2)	66(2)	72(2)	0(2)	29(2)	13(2)
C(12)	33(1)	54(2)	60(2)	8(1)	17(1)	13(1)
C(13)	26(1)	30(1)	41(1)	6(1)	8(1)	10(1)
C(14)	31(1)	38(1)	45(1)	1(1)	3(1)	12(1)
C(15)	39(1)	34(1)	58(2)	4(1)	13(1)	12(1)
C(16)	45(2)	38(2)	67(2)	20(1)	18(1)	18(1)
C(17)	52(2)	53(2)	45(2)	16(1)	4(1)	20(1)
C(18)	40(1)	39(1)	40(1)	6(1)	2(1)	11(1)

C(19)	29(1)	31(1)	32(1)	3(1)	12(1)	7(1)
C(20)	38(1)	44(2)	39(1)	1(1)	10(1)	16(1)
C(21)	54(2)	53(2)	57(2)	3(1)	20(2)	29(2)
C(22)	67(2)	60(2)	55(2)	-11(2)	26(2)	24(2)
C(23)	62(2)	68(2)	36(1)	-12(1)	10(1)	18(2)
C(24)	44(2)	46(2)	36(1)	-2(1)	8(1)	16(1)
C(25)	29(1)	35(1)	28(1)	2(1)	8(1)	14(1)
C(26)	33(1)	51(2)	40(1)	9(1)	8(1)	11(1)
C(27)	57(2)	65(2)	45(2)	22(1)	21(1)	19(2)
C(28)	68(2)	66(2)	29(1)	9(1)	9(1)	32(2)
C(29)	47(2)	64(2)	34(1)	-2(1)	-2(1)	22(1)
C(30)	33(1)	54(2)	34(1)	1(1)	6(1)	14(1)
C(31)	22(1)	35(1)	33(1)	6(1)	2(1)	9(1)
C(32)	29(1)	42(2)	42(1)	-2(1)	3(1)	7(1)
C(33)	37(1)	37(2)	48(2)	1(1)	-5(1)	2(1)
C(34)	36(1)	49(2)	49(2)	22(1)	-2(1)	-3(1)
C(35)	42(2)	57(2)	42(1)	17(1)	14(1)	6(1)
C(36)	36(1)	43(2)	35(1)	7(1)	9(1)	7(1)
C(37)	41(1)	27(1)	49(2)	2(1)	2(1)	5(1)
C(38)	43(2)	48(2)	52(2)	13(1)	-2(1)	6(1)
C(39)	54(2)	49(2)	48(2)	15(1)	3(1)	7(1)
C(40)	56(2)	40(2)	53(2)	7(1)	16(2)	5(1)
C(41)	40(2)	53(2)	53(2)	-1(1)	3(1)	-1(1)
C(42)	43(2)	46(2)	42(1)	1(1)	0(1)	5(1)
C(43)	74(2)	44(2)	57(2)	-2(1)	20(2)	3(2)
C(44)	56(2)	44(2)	90(2)	19(2)	22(2)	25(2)
C(45)	86(3)	95(3)	62(2)	23(2)	29(2)	13(2)
C(46)	24(2)	29(2)	53(3)	-8(2)	1(2)	9(2)
C(47)	31(2)	31(2)	81(3)	6(2)	0(2)	7(2)
C(48)	49(3)	34(3)	140(4)	4(3)	-9(3)	9(2)
C(49)	49(3)	32(3)	149(4)	-26(3)	-18(3)	11(2)
C(50)	50(2)	63(3)	96(3)	-38(2)	-15(3)	27(2)
C(51)	39(2)	60(3)	59(3)	-23(3)	-4(3)	21(2)
C(52)	47(3)	63(3)	83(3)	43(3)	21(3)	8(2)
C(53)	22(3)	30(3)	62(4)	-12(3)	12(3)	7(3)
C(54)	30(3)	35(3)	73(4)	-13(3)	10(3)	8(3)

C(55)	44(3)	26(3)	129(4)	-17(4)	6(4)	10(3)
C(56)	47(4)	27(4)	142(5)	-7(3)	13(4)	9(3)
C(57)	43(3)	39(3)	110(4)	20(3)	27(3)	10(3)
C(58)	36(3)	30(3)	76(4)	10(4)	21(4)	12(3)
C(59)	46(4)	71(4)	71(5)	-21(4)	7(4)	16(4)
O(3)	32(3)	41(3)	62(6)	14(3)	17(5)	14(3)

Table 16. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga71pas.

Atom	x	y	z	U(eq)
H(2)	5659	2322	1456	49
H(3)	4684	1052	202	65
H(4)	5461	931	-1005	69
H(5)	7216	2072	-985	68
H(6)	8242	3289	285	52
H(8)	8172	2780	3486	50
H(9)	7216	2320	4614	66
H(10)	5654	3020	4633	69
H(11)	4998	4096	3505	69
H(12)	5916	4536	2374	57
H(14)	8225	6166	2690	47
H(15)	7725	7765	2191	52
H(16)	6612	7784	711	58
H(17)	6009	6216	-281	60
H(18)	6519	4613	194	49
H(20)	13267	2535	3094	47
H(21)	13641	1228	2202	61
H(22)	12506	704	712	69
H(23)	11010	1507	110	67
H(24)	10630	2822	990	51
H(26)	10518	2726	3975	50
H(27)	11051	2167	5449	64

H(28)	12952	2697	6313	63
H(29)	14305	3830	5735	59
H(30)	13776	4415	4277	48
H(32)	12620	6069	3690	47
H(33)	14027	7591	3558	54
H(34)	15023	7524	2480	59
H(35)	14602	5962	1501	57
H(36)	13187	4439	1619	47
H(38)	9214	543	4218	62
H(39)	8041	-44	5159	64
H(41)	5284	-380	2988	63
H(42)	6467	219	2064	57
H(43A)	7509	460	894	90
H(43B)	8187	-473	1126	90
H(43C)	8732	607	704	90
H(44A)	10716	830	3340	91
H(44B)	10725	518	2319	91
H(44C)	10009	-345	2840	91
H(45A)	5597	-926	5886	121
H(45B)	6673	46	5873	121
H(45C)	6718	-1197	5719	121
H(48)	10937	7955	1960	97
H(49)	11157	8514	3484	103
H(50)	10791	7214	4514	90
H(51)	10205	5354	4021	66
H(52A)	9521	5523	848	97
H(52B)	10853	5569	1073	97
H(52C)	10410	6632	771	97
H(55)	10917	7816	3650	83
H(56)	11124	8599	2302	89
H(57)	10769	7482	964	75
H(58)	10206	5582	974	55
H(59A)	9536	5314	3863	97
H(59B)	10354	6431	4403	97
H(59C)	10883	5437	4228	97

X-Ray Crystal Structure of 10 (ga70fas).**Crystal data and structure refinement for ga70fas:**

Identification code	ga70fas	
Empirical formula	C50 H45 F3 Fe O2 P2 Pd Si	
Formula weight	987.14	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.8243(5) Å	a= 104.725(3)°.
	b = 11.9643(7) Å	b= 97.998(3)°.
	c = 20.2965(10) Å	g = 97.617(3)°.
Volume	2249.5(2) Å ³	
Z	2	
Density (calculated)	1.457 Mg/m ³	
Absorption coefficient	0.872 mm ⁻¹	
F(000)	1008	
Crystal size	0.10 x 0.10 x 0.03 mm ³	
Theta range for data collection	1.79 to 25.69°.	
Index ranges	-11<=h<=11, -14<=k<=14, -24<=l<=24	
Reflections collected	42149	
Independent reflections	8501 [R(int) = 0.0790]	
Completeness to theta = 25.69°	99.6 %	
Absorption correction	Integration	
Max. and min. transmission	0.97547 and 0.88858	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	8501 / 0 / 544	
Goodness-of-fit on F ²	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.0968	
R indices (all data)	R1 = 0.0857, wR2 = 0.1118	
Largest diff. peak and hole	1.116 and -0.655 e.Å ⁻³	

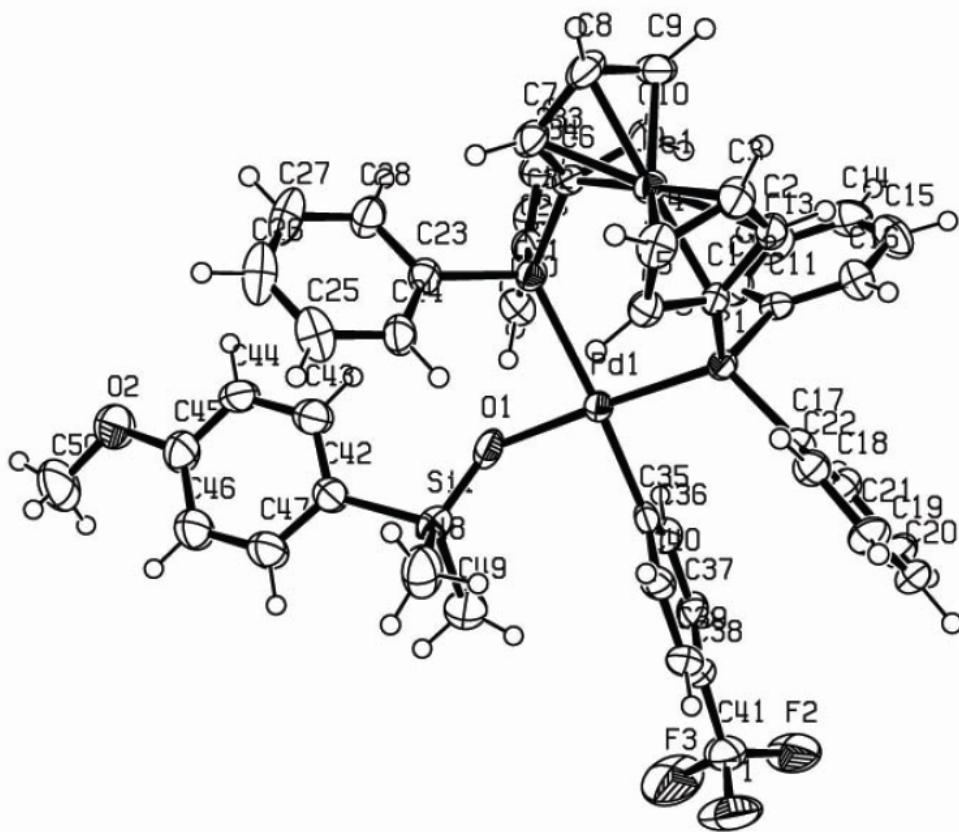


Figure 5. X-ray Structure of complex **10**.

X-ray quality crystals were obtained by vapor diffusion of pentane into a solution of 5 mg of **10** in 100 μ L of CH₂Cl₂. The crystals were obtained as an orange cube 0.10 x 0.10 x 0.03 in size and mounted using oil (Parantone-N, Exxon) to a thin glass fiber with the (1 0 0) scattering planes roughly normal to the spindle axis. Systematic absences for **10** were consistent with the space group P-1. Unit cell dimensions were $a = 9.8243(5)$ Å, $b = 11.9643(7)$ Å, $c = 20.2965(10)$ Å, $\alpha = 104.725(3)^\circ$, $\beta = 97.998(3)^\circ$, $\gamma = 97.617(3)^\circ$. Integration absorption correction was applied (absorption coefficient $\mu = 0.872$ mm⁻¹), and maximum and minimum transmission factors were 0.97547 and 0.88858. The 8501 data points were used in the full-matrix least-squares refinement. The structure was solved using direct methods by using SHELXTL software package. Hydrogen atoms were placed in “idealized” positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atom.

Table 17. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga70fas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	3173(4)	3078(4)	3881(2)	24(1)
C(2)	2854(5)	4200(4)	4218(2)	30(1)
C(3)	1464(5)	4008(4)	4341(2)	36(1)
C(4)	916(5)	2794(4)	4089(2)	37(1)
C(5)	1972(5)	2221(4)	3810(2)	30(1)
C(6)	1608(5)	2815(4)	2283(2)	30(1)
C(7)	192(5)	2710(4)	2375(2)	36(1)
C(8)	-76(5)	3841(5)	2690(2)	41(1)
C(9)	1157(5)	4657(5)	2786(2)	41(1)
C(10)	2212(5)	4046(4)	2541(2)	33(1)
C(11)	5655(4)	3929(4)	3381(2)	26(1)
C(12)	5856(5)	3802(4)	2705(2)	34(1)
C(13)	6508(5)	4736(5)	2513(3)	45(1)
C(14)	6969(6)	5815(5)	3004(3)	50(2)
C(15)	6814(6)	5936(5)	3676(3)	49(1)
C(16)	6140(5)	5007(4)	3867(2)	37(1)
C(17)	5809(4)	2696(4)	4419(2)	25(1)
C(18)	7263(5)	2848(4)	4500(2)	30(1)
C(19)	8048(5)	2773(4)	5106(2)	34(1)
C(20)	7419(5)	2550(4)	5631(2)	37(1)
C(21)	5987(5)	2405(4)	5561(2)	36(1)
C(22)	5175(5)	2475(4)	4957(2)	32(1)
C(23)	1016(5)	421(4)	1591(2)	32(1)
C(24)	681(5)	-417(4)	1922(2)	37(1)
C(25)	-526(6)	-1284(5)	1652(3)	55(2)
C(26)	-1360(6)	-1286(6)	1049(3)	60(2)
C(27)	-1029(6)	-458(6)	717(3)	58(2)
C(28)	149(5)	402(5)	979(2)	43(1)
C(29)	3294(5)	1936(4)	1281(2)	31(1)

C(30)	4288(5)	1281(4)	1042(2)	39(1)
C(31)	5004(6)	1578(5)	554(3)	48(1)
C(32)	4758(6)	2496(5)	304(3)	50(2)
C(33)	3765(6)	3140(5)	527(3)	50(2)
C(34)	3010(5)	2847(4)	1012(2)	39(1)
C(35)	5911(5)	491(4)	3197(2)	28(1)
C(36)	7151(5)	585(4)	2928(2)	32(1)
C(37)	8294(5)	150(4)	3179(2)	36(1)
C(38)	8226(5)	-404(4)	3696(2)	33(1)
C(39)	7022(5)	-491(4)	3977(2)	37(1)
C(40)	5884(5)	-43(4)	3731(2)	33(1)
C(41)	9446(6)	-914(5)	3927(3)	50(2)
F(1)	9267(4)	-1454(3)	4408(2)	83(1)
F(2)	10615(3)	-160(3)	4166(2)	91(1)
F(3)	9721(4)	-1755(4)	3410(2)	109(2)
C(42)	2809(5)	-2663(4)	970(2)	36(1)
C(43)	2206(6)	-2094(5)	517(3)	45(1)
C(44)	1472(6)	-2701(5)	-148(3)	47(1)
C(45)	1342(6)	-3889(5)	-379(3)	50(2)
C(46)	1896(7)	-4498(5)	56(3)	60(2)
C(47)	2611(6)	-3883(5)	721(3)	51(2)
C(48)	2990(6)	-2389(5)	2514(3)	58(2)
C(49)	5587(6)	-2329(5)	1889(3)	59(2)
C(50)	654(8)	-5624(5)	-1326(3)	76(2)
Fe(1)	1533(1)	3432(1)	3304(1)	28(1)
O(1)	3922(3)	-515(3)	1926(2)	38(1)
O(2)	647(5)	-4401(4)	-1041(2)	72(1)
P(1)	4746(1)	2681(1)	3601(1)	24(1)
P(2)	2506(1)	1592(1)	1989(1)	28(1)
Pd(1)	4276(1)	1037(1)	2727(1)	25(1)
Si(1)	3851(1)	-1820(1)	1856(1)	35(1)

Table 18. Bond lengths [\AA] and angles [$^\circ$] for ga70fas.

Atom	Bond lengths [\AA]	Atom	Bond angles [$^\circ$]
C(1)-C(5)	1.422(6)	C(5)-C(1)-C(2)	107.2(4)
C(1)-C(2)	1.439(6)	C(5)-C(1)-P(1)	121.8(3)
C(1)-P(1)	1.799(4)	C(2)-C(1)-P(1)	131.0(3)
C(1)-Fe(1)	2.014(4)	C(5)-C(1)-Fe(1)	70.2(2)
C(2)-C(3)	1.422(6)	C(2)-C(1)-Fe(1)	69.7(2)
C(2)-Fe(1)	2.028(4)	P(1)-C(1)-Fe(1)	126.8(2)
C(2)-H(2A)	1.0000	C(3)-C(2)-C(1)	107.6(4)
C(3)-C(4)	1.414(7)	C(3)-C(2)-Fe(1)	70.6(3)
C(3)-Fe(1)	2.055(4)	C(1)-C(2)-Fe(1)	68.6(2)
C(3)-H(3A)	1.0000	C(3)-C(2)-H(2A)	126.2
C(4)-C(5)	1.422(6)	C(1)-C(2)-H(2A)	126.2
C(4)-Fe(1)	2.062(5)	Fe(1)-C(2)-H(2A)	126.2
C(4)-H(4A)	1.0000	C(4)-C(3)-C(2)	108.7(4)
C(5)-Fe(1)	2.034(5)	C(4)-C(3)-Fe(1)	70.2(3)
C(5)-H(5A)	1.0000	C(2)-C(3)-Fe(1)	68.6(2)
C(6)-C(7)	1.422(6)	C(4)-C(3)-H(3A)	125.6
C(6)-C(10)	1.444(6)	C(2)-C(3)-H(3A)	125.6
C(6)-P(2)	1.823(4)	Fe(1)-C(3)-H(3A)	125.6
C(6)-Fe(1)	2.031(4)	C(3)-C(4)-C(5)	107.7(4)
C(7)-C(8)	1.417(7)	C(3)-C(4)-Fe(1)	69.6(3)
C(7)-Fe(1)	2.053(5)	C(5)-C(4)-Fe(1)	68.6(3)
C(7)-H(7A)	1.0000	C(3)-C(4)-H(4A)	126.1
C(8)-C(9)	1.408(7)	C(5)-C(4)-H(4A)	126.1
C(8)-Fe(1)	2.063(5)	Fe(1)-C(4)-H(4A)	126.1
C(8)-H(8A)	1.0000	C(4)-C(5)-C(1)	108.8(4)
C(9)-C(10)	1.419(6)	C(4)-C(5)-Fe(1)	70.7(3)
C(9)-Fe(1)	2.051(5)	C(1)-C(5)-Fe(1)	68.7(3)
C(9)-H(9A)	1.0000	C(4)-C(5)-H(5A)	125.6
C(10)-Fe(1)	2.030(5)	C(1)-C(5)-H(5A)	125.6
C(10)-H(10A)	1.0000	Fe(1)-C(5)-H(5A)	125.6
C(11)-C(12)	1.385(6)	C(7)-C(6)-C(10)	106.9(4)
C(11)-C(16)	1.388(6)	C(7)-C(6)-P(2)	125.3(4)
C(11)-P(1)	1.823(5)	C(10)-C(6)-P(2)	127.4(3)
C(12)-C(13)	1.383(7)	C(7)-C(6)-Fe(1)	70.5(3)

C(12)-H(12A)	0.9500	C(10)-C(6)-Fe(1)	69.1(2)
C(13)-C(14)	1.390(7)	P(2)-C(6)-Fe(1)	120.1(2)
C(13)-H(13A)	0.9500	C(8)-C(7)-C(6)	108.7(4)
C(14)-C(15)	1.368(7)	C(8)-C(7)-Fe(1)	70.2(3)
C(14)-H(14A)	0.9500	C(6)-C(7)-Fe(1)	68.8(3)
C(15)-C(16)	1.385(7)	C(8)-C(7)-H(7A)	125.6
C(15)-H(15A)	0.9500	C(6)-C(7)-H(7A)	125.6
C(16)-H(16A)	0.9500	Fe(1)-C(7)-H(7A)	125.6
C(17)-C(22)	1.394(6)	C(9)-C(8)-C(7)	108.0(4)
C(17)-C(18)	1.397(6)	C(9)-C(8)-Fe(1)	69.5(3)
C(17)-P(1)	1.829(4)	C(7)-C(8)-Fe(1)	69.5(3)
C(18)-C(19)	1.387(6)	C(9)-C(8)-H(8A)	126.0
C(18)-H(18A)	0.9500	C(7)-C(8)-H(8A)	126.0
C(19)-C(20)	1.370(6)	Fe(1)-C(8)-H(8A)	126.0
C(19)-H(19A)	0.9500	C(8)-C(9)-C(10)	108.8(4)
C(20)-C(21)	1.376(6)	C(8)-C(9)-Fe(1)	70.4(3)
C(20)-H(20A)	0.9500	C(10)-C(9)-Fe(1)	68.9(3)
C(21)-C(22)	1.393(6)	C(8)-C(9)-H(9A)	125.6
C(21)-H(21A)	0.9500	C(10)-C(9)-H(9A)	125.6
C(22)-H(22A)	0.9500	Fe(1)-C(9)-H(9A)	125.6
C(23)-C(24)	1.372(7)	C(9)-C(10)-C(6)	107.5(4)
C(23)-C(28)	1.397(6)	C(9)-C(10)-Fe(1)	70.5(3)
C(23)-P(2)	1.819(5)	C(6)-C(10)-Fe(1)	69.2(3)
C(24)-C(25)	1.409(7)	C(9)-C(10)-H(10A)	126.2
C(24)-H(24A)	0.9500	C(6)-C(10)-H(10A)	126.2
C(25)-C(26)	1.375(8)	Fe(1)-C(10)-H(10A)	126.2
C(25)-H(25A)	0.9500	C(12)-C(11)-C(16)	118.9(4)
C(26)-C(27)	1.362(8)	C(12)-C(11)-P(1)	119.1(4)
C(26)-H(26A)	0.9500	C(16)-C(11)-P(1)	122.0(3)
C(27)-C(28)	1.384(7)	C(13)-C(12)-C(11)	120.9(5)
C(27)-H(27A)	0.9500	C(13)-C(12)-H(12A)	119.6
C(28)-H(28A)	0.9500	C(11)-C(12)-H(12A)	119.6
C(29)-C(34)	1.380(6)	C(12)-C(13)-C(14)	119.5(5)
C(29)-C(30)	1.394(6)	C(12)-C(13)-H(13A)	120.2
C(29)-P(2)	1.834(4)	C(14)-C(13)-H(13A)	120.2
C(30)-C(31)	1.381(7)	C(15)-C(14)-C(13)	119.8(5)

C(30)-H(30A)	0.9500	C(15)-C(14)-H(14A)	120.1
C(31)-C(32)	1.358(7)	C(13)-C(14)-H(14A)	120.1
C(31)-H(31A)	0.9500	C(14)-C(15)-C(16)	120.6(5)
C(32)-C(33)	1.377(7)	C(14)-C(15)-H(15A)	119.7
C(32)-H(32A)	0.9500	C(16)-C(15)-H(15A)	119.7
C(33)-C(34)	1.397(7)	C(15)-C(16)-C(11)	120.2(5)
C(33)-H(33A)	0.9500	C(15)-C(16)-H(16A)	119.9
C(34)-H(34A)	0.9500	C(11)-C(16)-H(16A)	119.9
C(35)-C(40)	1.391(6)	C(22)-C(17)-C(18)	118.7(4)
C(35)-C(36)	1.406(6)	C(22)-C(17)-P(1)	120.4(3)
C(35)-Pd(1)	2.022(4)	C(18)-C(17)-P(1)	120.8(3)
C(36)-C(37)	1.387(6)	C(19)-C(18)-C(17)	120.1(4)
C(36)-H(36A)	0.9500	C(19)-C(18)-H(18A)	120.0
C(37)-C(38)	1.379(6)	C(17)-C(18)-H(18A)	120.0
C(37)-H(37A)	0.9500	C(20)-C(19)-C(18)	120.9(5)
C(38)-C(39)	1.386(7)	C(20)-C(19)-H(19A)	119.5
C(38)-C(41)	1.487(7)	C(18)-C(19)-H(19A)	119.5
C(39)-C(40)	1.388(6)	C(19)-C(20)-C(21)	119.7(4)
C(39)-H(39A)	0.9500	C(19)-C(20)-H(20A)	120.2
C(40)-H(40A)	0.9500	C(21)-C(20)-H(20A)	120.2
C(41)-F(2)	1.310(6)	C(20)-C(21)-C(22)	120.5(4)
C(41)-F(1)	1.319(6)	C(20)-C(21)-H(21A)	119.7
C(41)-F(3)	1.343(6)	C(22)-C(21)-H(21A)	119.7
C(42)-C(43)	1.390(7)	C(21)-C(22)-C(17)	120.1(4)
C(42)-C(47)	1.395(7)	C(21)-C(22)-H(22A)	119.9
C(42)-Si(1)	1.894(5)	C(17)-C(22)-H(22A)	119.9
C(43)-C(44)	1.399(7)	C(24)-C(23)-C(28)	119.2(5)
C(43)-H(43A)	0.9500	C(24)-C(23)-P(2)	119.3(4)
C(44)-C(45)	1.362(7)	C(28)-C(23)-P(2)	121.4(4)
C(44)-H(44A)	0.9500	C(23)-C(24)-C(25)	120.5(5)
C(45)-O(2)	1.364(6)	C(23)-C(24)-H(24A)	119.7
C(45)-C(46)	1.380(7)	C(25)-C(24)-H(24A)	119.7
C(46)-C(47)	1.396(7)	C(26)-C(25)-C(24)	119.2(6)
C(46)-H(46A)	0.9500	C(26)-C(25)-H(25A)	120.4
C(47)-H(47A)	0.9500	C(24)-C(25)-H(25A)	120.4
C(48)-Si(1)	1.895(5)	C(27)-C(26)-C(25)	120.5(6)

C(48)-H(48A)	0.9800	C(27)-C(26)-H(26A)	119.8
C(48)-H(48B)	0.9800	C(25)-C(26)-H(26A)	119.8
C(48)-H(48C)	0.9800	C(26)-C(27)-C(28)	120.9(5)
C(49)-Si(1)	1.884(5)	C(26)-C(27)-H(27A)	119.5
C(49)-H(49A)	0.9800	C(28)-C(27)-H(27A)	119.5
C(49)-H(49B)	0.9800	C(27)-C(28)-C(23)	119.7(5)
C(49)-H(49C)	0.9800	C(27)-C(28)-H(28A)	120.1
C(50)-O(2)	1.432(7)	C(23)-C(28)-H(28A)	120.1
C(50)-H(50A)	0.9800	C(34)-C(29)-C(30)	119.7(4)
C(50)-H(50B)	0.9800	C(34)-C(29)-P(2)	123.0(4)
C(50)-H(50C)	0.9800	C(30)-C(29)-P(2)	117.2(4)
O(1)-Si(1)	1.523(4)	C(31)-C(30)-C(29)	119.4(5)
O(1)-Pd(1)	2.085(3)	C(31)-C(30)-H(30A)	120.3
P(1)-Pd(1)	2.2336(12)	C(29)-C(30)-H(30A)	120.3
P(2)-Pd(1)	2.4060(12)	C(32)-C(31)-C(30)	121.2(5)
		C(32)-C(31)-H(31A)	119.4
		C(30)-C(31)-H(31A)	119.4
		C(31)-C(32)-C(33)	120.0(5)
		C(31)-C(32)-H(32A)	120.0
		C(33)-C(32)-H(32A)	120.0
		C(32)-C(33)-C(34)	120.0(5)
		C(32)-C(33)-H(33A)	120.0
		C(34)-C(33)-H(33A)	120.0
		C(29)-C(34)-C(33)	119.7(5)
		C(29)-C(34)-H(34A)	120.1
		C(33)-C(34)-H(34A)	120.1
		C(40)-C(35)-C(36)	117.4(4)
		C(40)-C(35)-Pd(1)	125.6(3)
		C(36)-C(35)-Pd(1)	116.8(3)
		C(37)-C(36)-C(35)	121.1(5)
		C(37)-C(36)-H(36A)	119.4
		C(35)-C(36)-H(36A)	119.4
		C(38)-C(37)-C(36)	120.3(4)
		C(38)-C(37)-H(37A)	119.8
		C(36)-C(37)-H(37A)	119.8
		C(37)-C(38)-C(39)	119.6(4)

C(37)-C(38)-C(41)	118.8(5)
C(39)-C(38)-C(41)	121.7(5)
C(38)-C(39)-C(40)	120.1(5)
C(38)-C(39)-H(39A)	119.9
C(40)-C(39)-H(39A)	119.9
C(39)-C(40)-C(35)	121.5(4)
C(39)-C(40)-H(40A)	119.3
C(35)-C(40)-H(40A)	119.3
F(2)-C(41)-F(1)	106.1(5)
F(2)-C(41)-F(3)	105.5(5)
F(1)-C(41)-F(3)	103.3(5)
F(2)-C(41)-C(38)	114.8(5)
F(1)-C(41)-C(38)	114.3(5)
F(3)-C(41)-C(38)	111.8(5)
C(43)-C(42)-C(47)	115.3(5)
C(43)-C(42)-Si(1)	121.7(4)
C(47)-C(42)-Si(1)	123.0(4)
C(42)-C(43)-C(44)	122.4(5)
C(42)-C(43)-H(43A)	118.8
C(44)-C(43)-H(43A)	118.8
C(45)-C(44)-C(43)	120.4(5)
C(45)-C(44)-H(44A)	119.8
C(43)-C(44)-H(44A)	119.8
C(44)-C(45)-O(2)	116.3(5)
C(44)-C(45)-C(46)	119.4(5)
O(2)-C(45)-C(46)	124.2(5)
C(45)-C(46)-C(47)	119.5(5)
C(45)-C(46)-H(46A)	120.2
C(47)-C(46)-H(46A)	120.2
C(42)-C(47)-C(46)	122.9(5)
C(42)-C(47)-H(47A)	118.6
C(46)-C(47)-H(47A)	118.6
Si(1)-C(48)-H(48A)	109.5
Si(1)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
Si(1)-C(48)-H(48C)	109.5

H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
Si(1)-C(49)-H(49A)	109.5
Si(1)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
Si(1)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
O(2)-C(50)-H(50A)	109.5
O(2)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
O(2)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(1)-Fe(1)-C(2)	41.71(16)
C(1)-Fe(1)-C(10)	108.80(18)
C(2)-Fe(1)-C(10)	110.14(19)
C(1)-Fe(1)-C(6)	109.79(16)
C(2)-Fe(1)-C(6)	139.23(18)
C(10)-Fe(1)-C(6)	41.64(18)
C(1)-Fe(1)-C(5)	41.13(17)
C(2)-Fe(1)-C(5)	69.06(18)
C(10)-Fe(1)-C(5)	137.51(18)
C(6)-Fe(1)-C(5)	110.18(18)
C(1)-Fe(1)-C(9)	137.3(2)
C(2)-Fe(1)-C(9)	110.4(2)
C(10)-Fe(1)-C(9)	40.69(18)
C(6)-Fe(1)-C(9)	68.89(18)
C(5)-Fe(1)-C(9)	178.05(19)
C(1)-Fe(1)-C(7)	139.88(17)
C(2)-Fe(1)-C(7)	178.1(2)
C(10)-Fe(1)-C(7)	68.66(19)
C(6)-Fe(1)-C(7)	40.75(17)
C(5)-Fe(1)-C(7)	112.8(2)
C(9)-Fe(1)-C(7)	67.7(2)
C(1)-Fe(1)-C(3)	69.15(17)

C(2)-Fe(1)-C(3)	40.75(17)
C(10)-Fe(1)-C(3)	139.8(2)
C(6)-Fe(1)-C(3)	178.28(19)
C(5)-Fe(1)-C(3)	68.12(18)
C(9)-Fe(1)-C(3)	112.8(2)
C(7)-Fe(1)-C(3)	139.35(19)
C(1)-Fe(1)-C(4)	69.10(18)
C(2)-Fe(1)-C(4)	68.59(19)
C(10)-Fe(1)-C(4)	177.88(19)
C(6)-Fe(1)-C(4)	138.32(19)
C(5)-Fe(1)-C(4)	40.62(17)
C(9)-Fe(1)-C(4)	141.16(19)
C(7)-Fe(1)-C(4)	112.7(2)
C(3)-Fe(1)-C(4)	40.18(19)
C(1)-Fe(1)-C(8)	177.1(2)
C(2)-Fe(1)-C(8)	138.05(19)
C(10)-Fe(1)-C(8)	68.3(2)
C(6)-Fe(1)-C(8)	68.62(18)
C(5)-Fe(1)-C(8)	141.5(2)
C(9)-Fe(1)-C(8)	40.0(2)
C(7)-Fe(1)-C(8)	40.28(18)
C(3)-Fe(1)-C(8)	112.50(19)
C(4)-Fe(1)-C(8)	113.8(2)
Si(1)-O(1)-Pd(1)	137.22(19)
C(45)-O(2)-C(50)	117.2(5)
C(1)-P(1)-C(11)	107.8(2)
C(1)-P(1)-C(17)	101.42(19)
C(11)-P(1)-C(17)	103.2(2)
C(1)-P(1)-Pd(1)	111.15(14)
C(11)-P(1)-Pd(1)	112.95(14)
C(17)-P(1)-Pd(1)	119.14(14)
C(23)-P(2)-C(6)	100.1(2)
C(23)-P(2)-C(29)	106.6(2)
C(6)-P(2)-C(29)	104.0(2)
C(23)-P(2)-Pd(1)	113.37(16)
C(6)-P(2)-Pd(1)	123.90(15)

C(29)-P(2)-Pd(1)	107.40(15)
C(35)-Pd(1)-O(1)	89.22(14)
C(35)-Pd(1)-P(1)	88.32(12)
O(1)-Pd(1)-P(1)	177.48(9)
C(35)-Pd(1)-P(2)	170.06(13)
O(1)-Pd(1)-P(2)	84.16(9)
P(1)-Pd(1)-P(2)	98.21(4)
O(1)-Si(1)-C(49)	114.9(2)
O(1)-Si(1)-C(42)	108.0(2)
C(49)-Si(1)-C(42)	105.2(2)
O(1)-Si(1)-C(48)	115.8(2)
C(49)-Si(1)-C(48)	105.3(3)
C(42)-Si(1)-C(48)	106.9(2)

Table 19. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga70fas. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^*{}^2 U^{11} + \dots + 2hka^*b^*U^{12}]$

Atom	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	21(2)	25(2)	21(2)	4(2)	0(2)	2(2)
C(2)	29(3)	31(3)	26(2)	3(2)	1(2)	5(2)
C(3)	31(3)	42(3)	30(3)	1(2)	8(2)	11(2)
C(4)	29(3)	47(3)	34(3)	10(2)	12(2)	3(2)
C(5)	30(3)	33(3)	27(2)	10(2)	5(2)	4(2)
C(6)	29(3)	32(3)	28(2)	10(2)	0(2)	9(2)
C(7)	23(3)	42(3)	37(3)	4(2)	0(2)	9(2)
C(8)	28(3)	55(4)	36(3)	5(3)	-3(2)	16(3)
C(9)	49(3)	38(3)	38(3)	9(2)	1(3)	23(3)
C(10)	39(3)	33(3)	28(2)	10(2)	3(2)	5(2)
C(11)	24(2)	28(3)	29(2)	14(2)	5(2)	7(2)
C(12)	27(3)	39(3)	36(3)	14(2)	3(2)	0(2)
C(13)	35(3)	64(4)	45(3)	30(3)	8(3)	4(3)
C(14)	42(3)	41(4)	76(4)	36(3)	11(3)	0(3)
C(15)	47(3)	32(3)	67(4)	11(3)	16(3)	-1(3)
C(16)	39(3)	32(3)	37(3)	5(2)	11(2)	3(2)
C(17)	29(3)	20(2)	27(2)	5(2)	6(2)	5(2)
C(18)	30(3)	35(3)	24(2)	5(2)	5(2)	8(2)
C(19)	29(3)	40(3)	33(3)	8(2)	-2(2)	10(2)
C(20)	41(3)	38(3)	30(3)	8(2)	-6(2)	12(2)
C(21)	44(3)	45(3)	26(2)	20(2)	6(2)	8(3)
C(22)	32(3)	32(3)	34(3)	13(2)	6(2)	3(2)
C(23)	30(3)	32(3)	31(3)	0(2)	4(2)	8(2)
C(24)	38(3)	33(3)	33(3)	1(2)	2(2)	2(2)
C(25)	60(4)	42(4)	52(4)	2(3)	15(3)	-7(3)
C(26)	46(4)	68(5)	47(4)	-5(3)	5(3)	-17(3)
C(27)	43(4)	78(5)	35(3)	-3(3)	-6(3)	-5(3)
C(28)	40(3)	46(3)	36(3)	5(3)	-4(3)	4(3)
C(29)	36(3)	32(3)	23(2)	8(2)	3(2)	3(2)
C(30)	45(3)	33(3)	39(3)	8(2)	10(2)	7(2)
C(31)	54(4)	47(4)	50(3)	15(3)	22(3)	15(3)
C(32)	57(4)	59(4)	40(3)	19(3)	17(3)	7(3)
C(33)	69(4)	48(4)	35(3)	17(3)	7(3)	15(3)

C(34)	45(3)	44(3)	29(3)	10(2)	7(2)	16(3)
C(35)	25(3)	19(2)	33(3)	-3(2)	2(2)	1(2)
C(36)	28(3)	35(3)	32(3)	7(2)	7(2)	5(2)
C(37)	25(3)	37(3)	39(3)	4(2)	1(2)	4(2)
C(38)	27(3)	27(3)	39(3)	8(2)	-9(2)	4(2)
C(39)	42(3)	29(3)	41(3)	16(2)	0(2)	6(2)
C(40)	35(3)	27(3)	38(3)	13(2)	7(2)	3(2)
C(41)	38(3)	45(4)	69(4)	23(3)	-2(3)	9(3)
F(1)	55(2)	92(3)	125(3)	74(3)	0(2)	23(2)
F(2)	35(2)	70(3)	167(4)	61(3)	-28(2)	-5(2)
F(3)	98(3)	121(4)	104(3)	4(3)	-2(3)	84(3)
C(42)	40(3)	31(3)	37(3)	9(2)	6(2)	6(2)
C(43)	53(3)	39(3)	44(3)	12(3)	6(3)	14(3)
C(44)	59(4)	42(3)	39(3)	10(3)	-5(3)	20(3)
C(45)	62(4)	45(4)	36(3)	10(3)	-5(3)	0(3)
C(46)	86(5)	40(4)	44(3)	7(3)	-11(3)	7(3)
C(47)	73(4)	37(3)	42(3)	14(3)	1(3)	10(3)
C(48)	71(4)	58(4)	37(3)	11(3)	3(3)	-8(3)
C(49)	55(4)	49(4)	68(4)	8(3)	0(3)	20(3)
C(50)	117(6)	47(4)	47(4)	-2(3)	-5(4)	0(4)
Fe(1)	24(1)	31(1)	28(1)	5(1)	3(1)	8(1)
O(1)	33(2)	44(2)	29(2)	11(2)	-8(2)	-6(2)
O(2)	102(4)	52(3)	44(2)	0(2)	-23(2)	11(2)
P(1)	22(1)	26(1)	22(1)	6(1)	2(1)	5(1)
P(2)	28(1)	30(1)	24(1)	5(1)	2(1)	6(1)
Pd(1)	24(1)	24(1)	25(1)	4(1)	2(1)	5(1)
Si(1)	33(1)	41(1)	29(1)	10(1)	2(1)	7(1)

Table 20. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ga70fas.

Atom	x	y	z	U(eq)
H(2A)	3495	4974	4342	36
H(3A)	949	4632	4556	43
H(4A)	-48	2410	4096	44
H(5A)	1878	1359	3590	36
H(7A)	-493	1960	2251	43

H(8A)	-979	4025	2826	50
H(9A)	1277	5522	3001	50
H(10A)	3191	4404	2541	40
H(12A)	5541	3064	2370	41
H(13A)	6641	4640	2048	54
H(14A)	7390	6468	2873	60
H(15A)	7172	6663	4016	59
H(16A)	6010	5109	4333	44
H(18A)	7715	3004	4141	36
H(19A)	9037	2877	5157	41
H(20A)	7967	2497	6043	45
H(21A)	5550	2255	5926	44
H(22A)	4188	2371	4913	38
H(24A)	1268	-414	2337	45
H(25A)	-761	-1859	1884	65
H(26A)	-2173	-1870	861	72
H(27A)	-1614	-470	301	70
H(28A)	368	976	744	52
H(30A)	4471	637	1213	47
H(31A)	5681	1132	391	57
H(32A)	5272	2695	-26	60
H(33A)	3594	3783	352	59
H(34A)	2303	3274	1157	47
H(36A)	7207	953	2567	39
H(37A)	9127	233	2995	43
H(39A)	6976	-858	4339	44
H(40A)	5069	-102	3931	39
H(43A)	2295	-1264	664	54
H(44A)	1062	-2281	-439	57
H(46A)	1791	-5329	-96	72
H(47A)	2980	-4314	1016	61
H(48A)	1997	-2332	2442	87
H(48B)	3439	-1919	2982	87
H(48C)	3087	-3211	2458	87
H(49A)	6125	-2003	1589	88
H(49B)	5435	-3189	1730	88

H(49C)	6104	-2062	2366	88
H(50A)	239	-5862	-1819	114
H(50B)	111	-6081	-1083	114
H(50C)	1618	-5766	-1271	114

X-Ray Crystal Structure of 18 (ba80gas)**Crystal Data and Structure Refinement for ba80gas:**

Identification code	ba80gas		
Empirical formula	C ₂₇ H ₄₄ F O ₂ PdSi		
Formula weight	585.08		
Temperature	193(2) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	C2/c		
Unit cell dimensions	a = 25.0154(13) Å	a= 90°.	
	b = 11.3144(6) Å	b= 109.649(2)°.	
	c = 22.0186(11) Å	g = 90°.	
Volume	5869.1(5) Å ³		
Z	8		
Density (calculated)	1.324 Mg/m ³		
Absorption coefficient	0.754 mM ⁻¹		
F(000)	2448		
Crystal size	0.266 x 0.14 x 0.123 mm ³		
Theta range for data collection	1.96 to 25.39°.		
Index ranges	-30<=h<=30, -13<=k<=13, -26<=l<=26		
Reflections collected	48461		
Independent reflections	5412 [R(int) = 0.0613]		
Completeness to theta = 25.39°	99.9 %		
Absorption correction	Integration		
Max. and min. transmission	0.9473 and 0.8649		
Refinement method	Full-matrix least-squares on F ²		
Data / restraints / parameters	5412 / 0 / 310		
Goodness-of-fit on F ²	1.029		
Final R indices [I>2sigma(I)]	R1 = 0.0281, wR2 = 0.0611		
R indices (all data)	R1 = 0.0429, wR2 = 0.0668		
Largest diff. peak and hole	0.369 and -0.280 e.Å ⁻³		

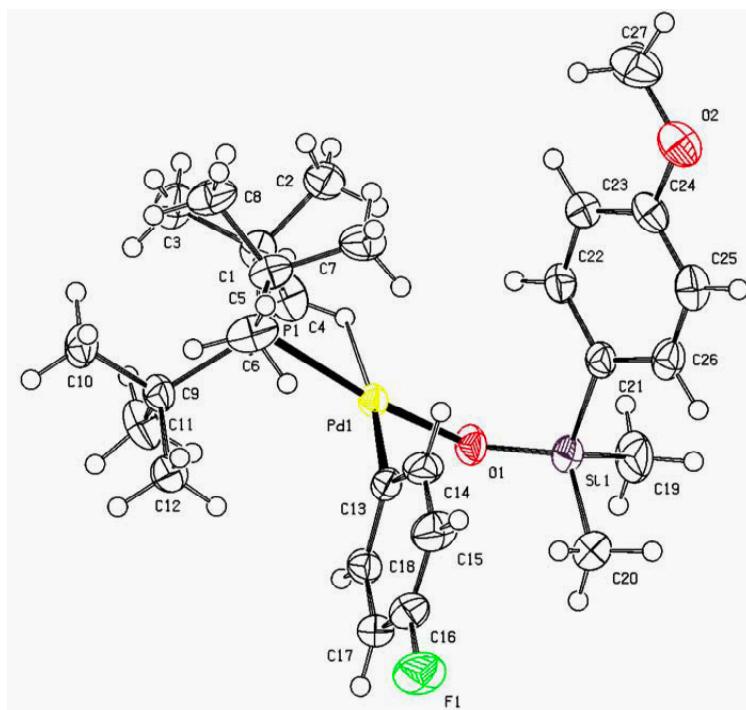


Figure 6. X-ray crystal structure of complex **18**.

The crystals were obtained directly from recrystallization (pentanes) as yellow needles $0.27 \times 0.14 \times 0.12$ mM in size and mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (0 -1 1) scattering planes roughly normal to the spindle axis. Systematic absences for **18** were consistent with the space group C2/c. Unit cell dimensions were $a = 25.0154(13)$ Å, $b = 11.3144(6)$ Å, $c = 22.0186(11)$ Å, $\alpha = 90.00^\circ$, $\beta = 109.649(2)^\circ$, $\gamma = 90.00^\circ$. Integration absorption correction was applied (absorption coefficient $\mu = 0.754$ mM⁻¹), and maximum and minimum transmission factors were 0.9473 and 0.8649. The 5412 data points were used in the full-matrix least-squares refinement. The structure was solved using direct methods by using SHELXTL software package. A structural model consisting of the host molecule was developed. Methyl H atom positions, R-CH~3~, were optimized by rotation about R-C bonds with idealized C-H, R--H and H--H distances. Remaining H atoms were included as riding idealized contributors. Methyl H atom U's were assigned as 1.5 times U~eq~ of the carrier atom;

remaining H atom U's were assigned as 1.2 times carrier U_{eq}.

Table 21. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ba80gas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Pd(1)	1128(1)	1928(1)	635(1)	27(1)
P(1)	1226(1)	3287(1)	1417(1)	26(1)
Si(1)	1429(1)	-77(1)	-269(1)	37(1)
F(1)	525(1)	-2489(2)	1831(1)	62(1)
O(1)	1069(1)	1046(2)	-181(1)	36(1)
O(2)	3919(1)	513(2)	1343(1)	47(1)
C(1)	1418(1)	4552(2)	957(1)	34(1)
C(2)	2043(1)	4482(3)	1001(1)	41(1)
C(3)	1310(1)	5809(2)	1151(2)	48(1)
C(4)	1074(1)	4339(3)	238(1)	44(1)
C(5)	1824(1)	3090(2)	2214(1)	36(1)
C(6)	1627(1)	2282(3)	2662(1)	45(1)
C(7)	2323(1)	2466(3)	2086(2)	44(1)
C(8)	2037(1)	4247(3)	2579(1)	47(1)
C(9)	539(1)	3654(2)	1567(1)	34(1)
C(10)	598(1)	4596(3)	2088(2)	48(1)
C(11)	95(1)	4065(3)	931(2)	50(1)
C(12)	292(1)	2529(3)	1764(2)	44(1)
C(13)	965(1)	528(2)	1071(1)	29(1)
C(14)	1371(1)	-118(2)	1536(2)	41(1)
C(15)	1222(1)	-1134(2)	1792(2)	48(1)
C(16)	669(1)	-1495(2)	1571(2)	42(1)
C(17)	258(1)	-910(2)	1095(1)	38(1)
C(18)	412(1)	110(2)	845(1)	32(1)
C(19)	1404(1)	-134(3)	-1129(2)	59(1)
C(20)	1164(1)	-1533(3)	-86(2)	54(1)
C(21)	2195(1)	75(2)	258(1)	32(1)
C(22)	2427(1)	1190(2)	435(1)	37(1)
C(23)	2992(1)	1391(3)	797(1)	37(1)

C(24)	3352(1)	429(3)	994(1)	35(1)
C(25)	3139(1)	-698(3)	828(1)	39(1)
C(26)	2576(1)	-868(2)	471(1)	37(1)
C(27)	4144(1)	1670(3)	1525(2)	58(1)

Table 22. Bond lengths [Å] and angles [°] for ba80gas.

Pd(1)-C(13)	1.965(3)
Pd(1)-O(1)	2.0163(17)
Pd(1)-P(1)	2.2591(7)
P(1)-C(5)	1.898(3)
P(1)-C(9)	1.902(3)
P(1)-C(1)	1.906(3)
Si(1)-O(1)	1.6063(19)
Si(1)-C(20)	1.870(3)
Si(1)-C(19)	1.875(3)
Si(1)-C(21)	1.884(3)
F(1)-C(16)	1.365(3)
O(2)-C(24)	1.370(3)
O(2)-C(27)	1.429(4)
C(1)-C(3)	1.534(4)
C(1)-C(2)	1.536(4)
C(1)-C(4)	1.547(4)
C(2)-H(2A)	0.9800
C(2)-H(30i)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(31i)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(8)	1.535(4)
C(5)-C(7)	1.540(4)
C(5)-C(6)	1.542(4)

C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.536(4)
C(9)-C(11)	1.537(4)
C(9)-C(12)	1.539(4)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(130i)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.383(4)
C(13)-C(18)	1.387(3)
C(14)-C(15)	1.385(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.365(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.367(4)
C(17)-C(18)	1.387(4)
C(17)-H(31o)	0.9500
C(18)-H(18A)	0.9500
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800

C(20)-H(31j)	0.9800
C(21)-C(22)	1.388(4)
C(21)-C(26)	1.402(4)
C(22)-C(23)	1.389(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.385(4)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.382(4)
C(25)-C(26)	1.377(4)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(13)-Pd(1)-O(1)	94.08(9)
C(13)-Pd(1)-P(1)	99.39(7)
O(1)-Pd(1)-P(1)	166.51(6)
C(5)-P(1)-C(9)	110.02(12)
C(5)-P(1)-C(1)	108.50(12)
C(9)-P(1)-C(1)	109.44(12)
C(5)-P(1)-Pd(1)	118.29(9)
C(9)-P(1)-Pd(1)	114.15(9)
C(1)-P(1)-Pd(1)	95.08(8)
O(1)-Si(1)-C(20)	114.71(12)
O(1)-Si(1)-C(19)	108.58(13)
C(20)-Si(1)-C(19)	107.09(16)
O(1)-Si(1)-C(21)	110.38(11)
C(20)-Si(1)-C(21)	108.01(14)
C(19)-Si(1)-C(21)	107.82(13)
Si(1)-O(1)-Pd(1)	128.52(11)
C(24)-O(2)-C(27)	117.2(2)
C(3)-C(1)-C(2)	107.6(2)
C(3)-C(1)-C(4)	109.9(2)
C(2)-C(1)-C(4)	105.1(2)
C(3)-C(1)-P(1)	116.67(18)

C(2)-C(1)-P(1)	111.21(18)
C(4)-C(1)-P(1)	105.89(19)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(30i)	109.5
H(2A)-C(2)-H(30i)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(30i)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(31i)	109.5
H(3A)-C(3)-H(31i)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(31i)-C(3)-H(3C)	109.5
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(8)-C(5)-C(7)	109.0(2)
C(8)-C(5)-C(6)	107.5(2)
C(7)-C(5)-C(6)	107.4(2)
C(8)-C(5)-P(1)	114.23(19)
C(7)-C(5)-P(1)	108.71(19)
C(6)-C(5)-P(1)	109.79(19)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5

H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(11)	109.2(2)
C(10)-C(9)-C(12)	108.1(2)
C(11)-C(9)-C(12)	105.7(2)
C(10)-C(9)-P(1)	114.6(2)
C(11)-C(9)-P(1)	108.98(18)
C(12)-C(9)-P(1)	109.86(19)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(130i)	109.5
H(12A)-C(12)-H(130i)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(130i)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	118.7(2)
C(14)-C(13)-Pd(1)	124.5(2)
C(18)-C(13)-Pd(1)	116.47(19)
C(13)-C(14)-C(15)	120.6(3)

C(13)-C(14)-H(14A)	119.7
C(15)-C(14)-H(14A)	119.7
C(16)-C(15)-C(14)	118.8(3)
C(16)-C(15)-H(15A)	120.6
C(14)-C(15)-H(15A)	120.6
C(15)-C(16)-F(1)	118.5(3)
C(15)-C(16)-C(17)	122.6(3)
F(1)-C(16)-C(17)	118.9(3)
C(16)-C(17)-C(18)	118.0(3)
C(16)-C(17)-H(31o)	121.0
C(18)-C(17)-H(31o)	121.0
C(13)-C(18)-C(17)	121.2(3)
C(13)-C(18)-H(18A)	119.4
C(17)-C(18)-H(18A)	119.4
Si(1)-C(19)-H(19A)	109.5
Si(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
Si(1)-C(20)-H(20A)	109.5
Si(1)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(1)-C(20)-H(31j)	109.5
H(20A)-C(20)-H(31j)	109.5
H(20B)-C(20)-H(31j)	109.5
C(22)-C(21)-C(26)	115.1(3)
C(22)-C(21)-Si(1)	119.9(2)
C(26)-C(21)-Si(1)	124.9(2)
C(21)-C(22)-C(23)	124.0(3)
C(21)-C(22)-H(22A)	118.0
C(23)-C(22)-H(22A)	118.0
C(24)-C(23)-C(22)	118.7(3)
C(24)-C(23)-H(23A)	120.7
C(22)-C(23)-H(23A)	120.7
O(2)-C(24)-C(25)	116.5(2)

O(2)-C(24)-C(23)	124.2(3)
C(25)-C(24)-C(23)	119.4(3)
C(26)-C(25)-C(24)	120.6(3)
C(26)-C(25)-H(25A)	119.7
C(24)-C(25)-H(25A)	119.7
C(25)-C(26)-C(21)	122.3(3)
C(25)-C(26)-H(26A)	118.9
C(21)-C(26)-H(26A)	118.9
O(2)-C(27)-H(27A)	109.5
O(2)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(2)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 23. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ba80gas. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

Atom	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pd(1)	26(1)	30(1)	26(1)	-4(1)	9(1)	1(1)
P(1)	30(1)	26(1)	22(1)	0(1)	11(1)	0(1)
Si(1)	37(1)	38(1)	38(1)	-13(1)	16(1)	-1(1)
F(1)	66(1)	37(1)	83(2)	15(1)	27(1)	-7(1)
O(1)	35(1)	44(1)	29(1)	-9(1)	12(1)	4(1)
O(2)	35(1)	61(1)	40(1)	8(1)	8(1)	7(1)
C(1)	45(2)	31(1)	30(2)	6(1)	19(1)	1(1)
C(2)	47(2)	39(2)	45(2)	3(1)	24(2)	-7(1)
C(3)	70(2)	31(2)	56(2)	7(1)	36(2)	2(2)
C(4)	50(2)	56(2)	31(2)	14(1)	20(1)	10(2)
C(5)	42(2)	35(2)	26(1)	2(1)	5(1)	-8(1)
C(6)	56(2)	41(2)	31(2)	7(1)	5(1)	-13(1)
C(7)	33(2)	43(2)	47(2)	6(2)	1(1)	-3(1)
C(8)	58(2)	46(2)	33(2)	-5(1)	10(2)	-19(2)

C(9)	37(2)	37(2)	35(2)	-2(1)	20(1)	1(1)
C(10)	63(2)	41(2)	56(2)	-9(2)	41(2)	-2(2)
C(11)	37(2)	66(2)	51(2)	6(2)	19(2)	15(2)
C(12)	45(2)	47(2)	48(2)	-11(2)	28(2)	-9(2)
C(13)	29(1)	27(1)	30(1)	-5(1)	9(1)	1(1)
C(14)	25(2)	33(2)	56(2)	-3(1)	2(1)	-1(1)
C(15)	43(2)	32(2)	57(2)	8(2)	3(2)	4(1)
C(16)	45(2)	29(1)	53(2)	1(1)	18(2)	-4(1)
C(17)	32(2)	36(2)	47(2)	-8(1)	14(1)	-6(1)
C(18)	27(1)	36(2)	31(2)	-3(1)	7(1)	1(1)
C(19)	58(2)	78(2)	44(2)	-25(2)	21(2)	4(2)
C(20)	48(2)	41(2)	76(2)	-18(2)	27(2)	-7(2)
C(21)	38(2)	32(1)	33(2)	-2(1)	21(1)	1(1)
C(22)	35(2)	34(2)	45(2)	-2(1)	18(1)	6(1)
C(23)	36(2)	35(2)	43(2)	-4(1)	18(1)	-2(1)
C(24)	31(2)	51(2)	25(1)	7(1)	13(1)	5(1)
C(25)	46(2)	38(2)	36(2)	9(1)	19(1)	12(1)
C(26)	51(2)	34(2)	34(2)	-1(1)	23(1)	3(1)
C(27)	39(2)	75(3)	51(2)	-1(2)	5(2)	-7(2)

Table 24. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ba80gas.

Atom	x	y	z	U(eq)
H(2A)	2108	5019	683	62
H(30i)	2133	3671	912	62
H(2C)	2287	4712	1435	62
H(3A)	1450	6384	907	72
H(31i)	1510	5921	1614	72
H(3C)	902	5925	1057	72
H(4A)	1148	4982	-22	66
H(4B)	668	4316	179	66
H(4C)	1188	3585	100	66
H(6A)	1951	2096	3048	68

H(6B)	1470	1549	2434	68
H(6C)	1334	2688	2787	68
H(7A)	2578	2128	2490	66
H(7B)	2532	3039	1918	66
H(7C)	2177	1834	1769	66
H(8A)	2329	4071	2994	70
H(8B)	1719	4658	2653	70
H(8C)	2198	4752	2322	70
H(10A)	221	4805	2099	72
H(10B)	780	5302	1988	72
H(10C)	830	4284	2509	72
H(11A)	-276	4137	988	75
H(11B)	70	3485	592	75
H(11C)	207	4833	808	75
H(12A)	-71	2716	1820	66
H(130i)	558	2226	2170	66
H(12C)	232	1929	1427	66
H(14A)	1755	137	1681	49
H(15A)	1500	-1571	2116	57
H(31o)	-121	-1192	941	46
H(18A)	133	530	514	38
H(19A)	1562	598	-1235	89
H(19B)	1009	-220	-1413	89
H(19C)	1627	-809	-1188	89
H(20A)	1176	-1542	364	80
H(20B)	1405	-2169	-153	80
H(31j)	772	-1653	-372	80
H(22A)	2184	1855	302	44
H(23A)	3130	2172	906	44
H(25A)	3384	-1361	962	46
H(26A)	2440	-1652	364	45
H(27A)	4554	1616	1754	86
H(27B)	3959	2031	1807	86
H(27C)	4074	2157	1137	86